

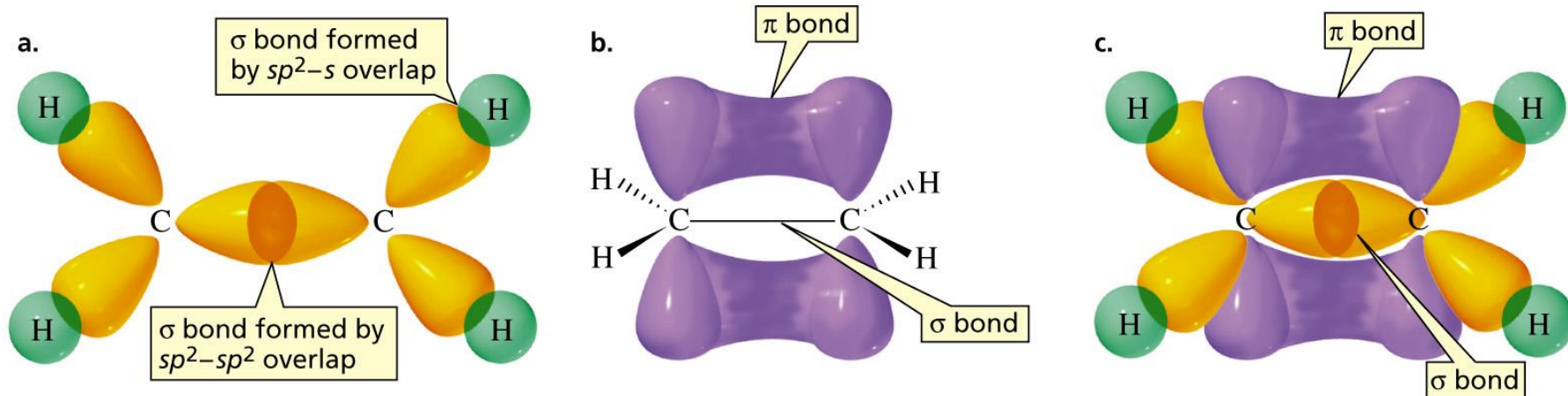
Chapter 1:
Electronic Structure and Bonding
Or

A Brief Review of General Chemistry

Part 2: Quantum Mechanics and
Molecular Orbital Theory

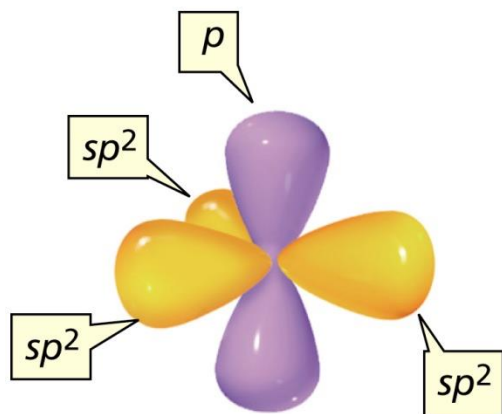
Review ideas from general chemistry:
atoms, bonds, molecular geometry

Hybrid Orbitals of Ethene, C_2H_4

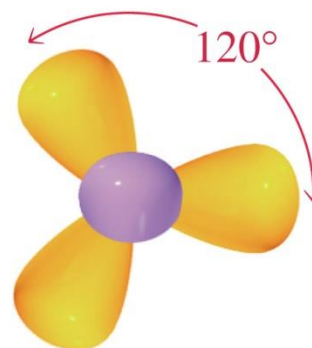


Bonding in Ethene (Ethylene): A Double Bond

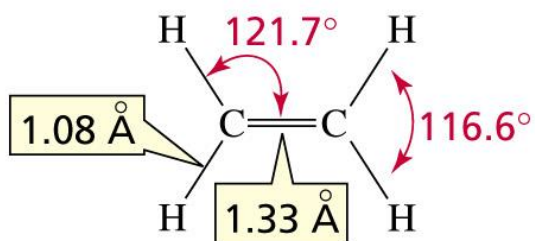
Hybrid Orbitals of Ethene, C_2H_4



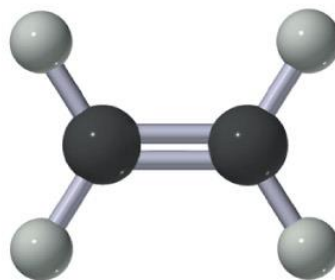
side view



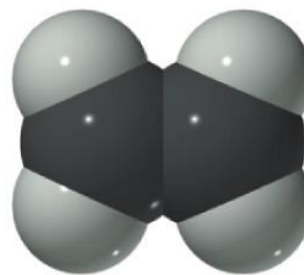
top view



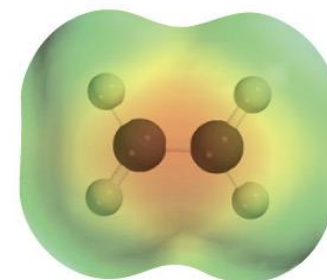
a double bond consists of one σ bond and one π bond



ball-and-stick model of ethene



space-filling model of ethene



electrostatic potential map for ethene

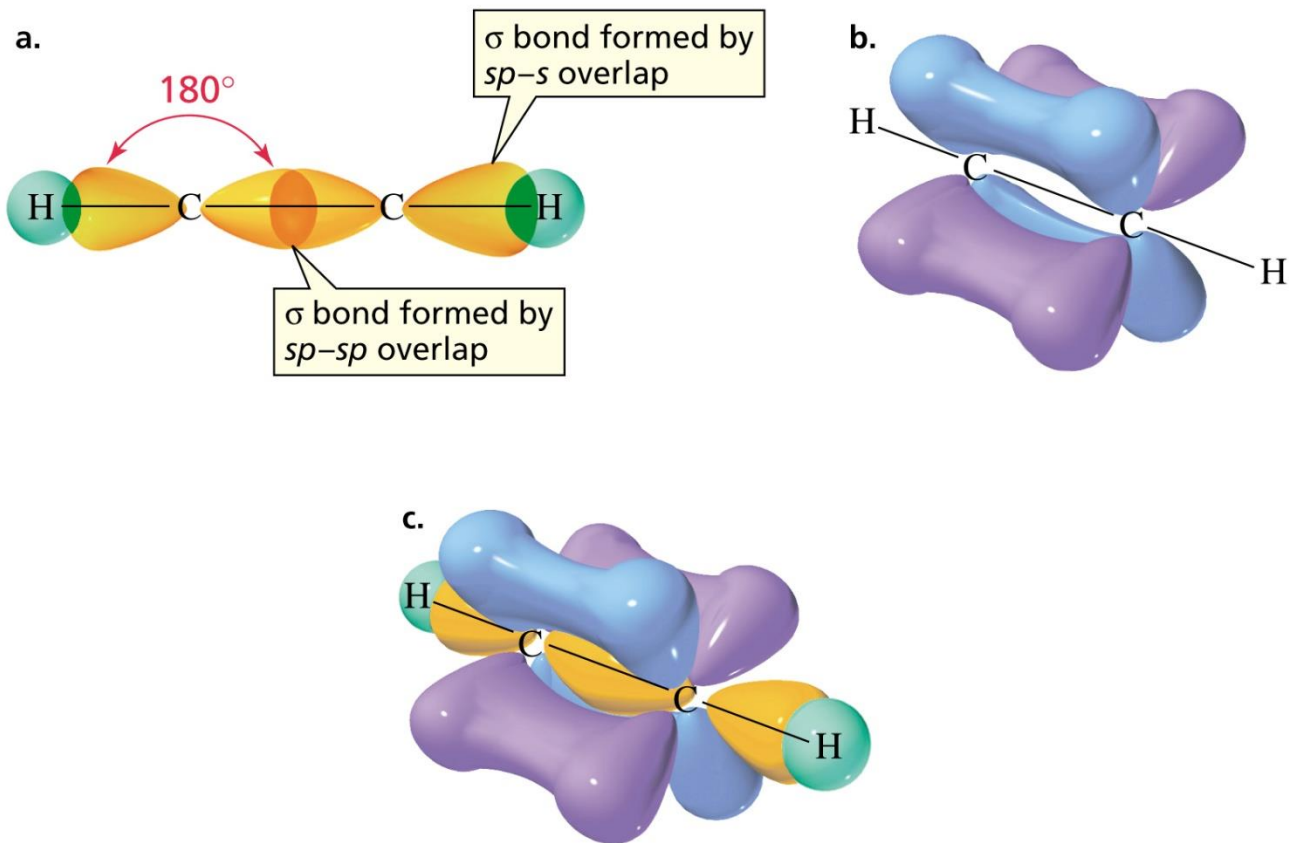
Molecular Orbital Theory

So let's look at Ethyne (Acetylene) . . .

CHCH

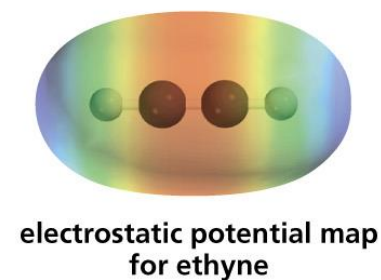
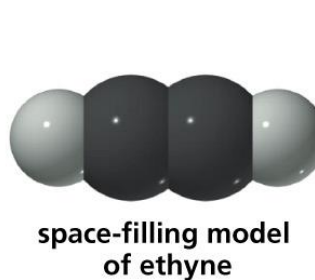
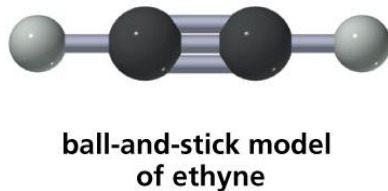
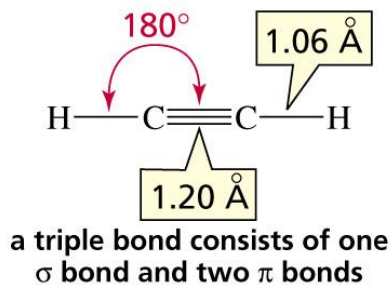
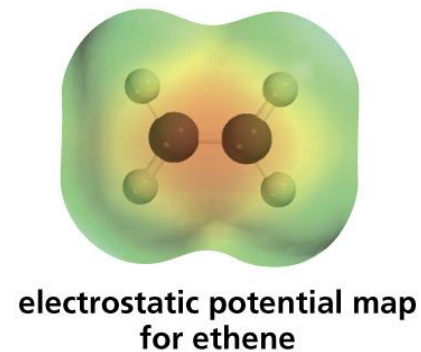
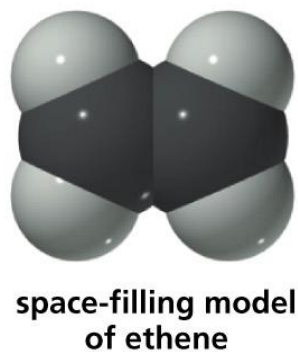
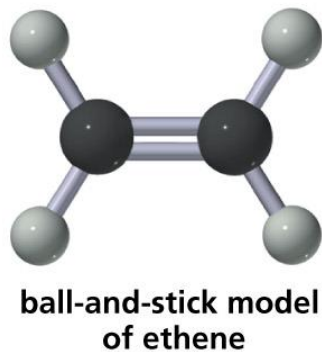
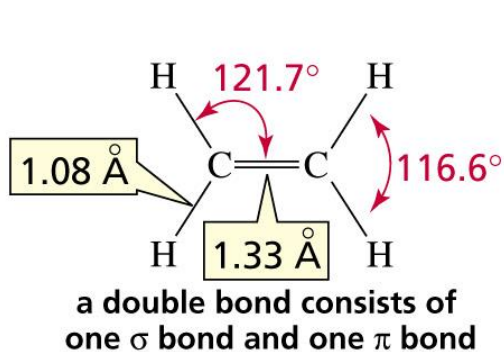
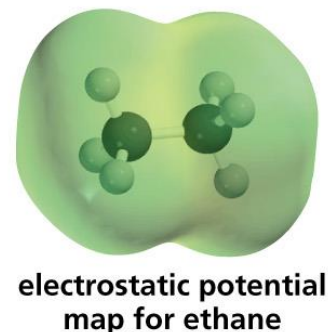
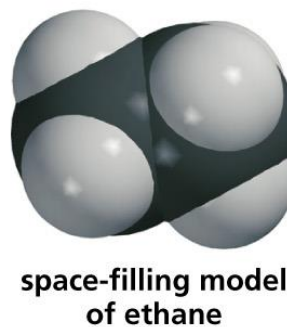
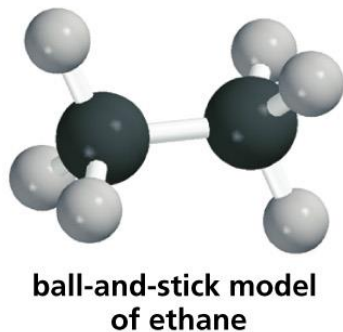
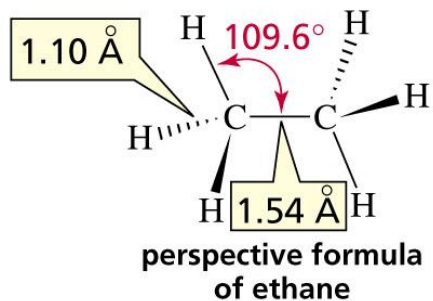
Draw a Lewis Dot Structure for Ethyne

Hybrid Orbitals of Ethyne, C_2H_2



Bonding in Ethyne (Acetylene) : A Triple Bond

Molecular Orbital Theory



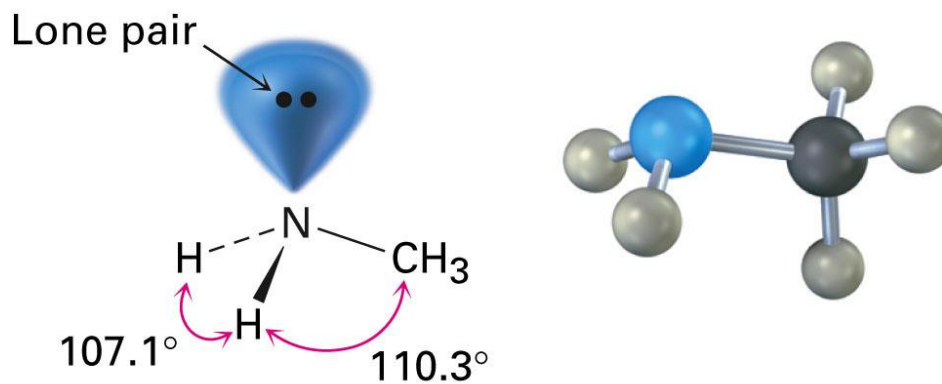
Molecular Orbital Theory

Summary

- ▶ The sharing of **one** pair of electrons is a **single** bond.
- ▶ The sharing of **two** pairs gives a **double** bond.
- ▶ The sharing of **three** pairs gives a **triple** bond.

Hybridization of Nitrogen and Oxygen

Elements other than C can have hybridized orbitals



Methylamine

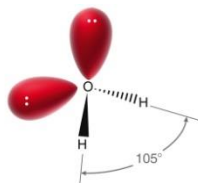
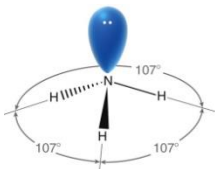
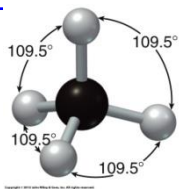
Chapter 2:
Molecular Representations
Chapter 2 (2.1-2.7)

Or

Functional Groups and Resonance
(Atoms First!: *Sections 6.4 and 6.5, 7.1- 7.8, 23.1-23.3*)

Molecular Geometry – sp^3 Geometry

Example	Steric number	Hybridization	Arrangement of electron pairs	Arrangement of atoms (geometry)
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Representing Molecules

Bonding Models (C₂H₄O₂)

▶ Lewis Dot structures

- There are many ways to represent molecules.

▶ Line structures

- If you were representing a large molecule with 20 or more atoms, which structure would be most time consuming to draw?

▶ Condensed structures

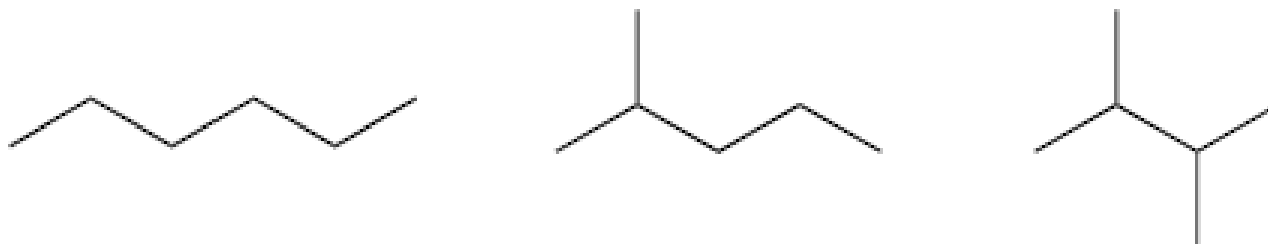


- Which structures give you the most information about the structure?

▶ Organic structures

Bond-line Structures

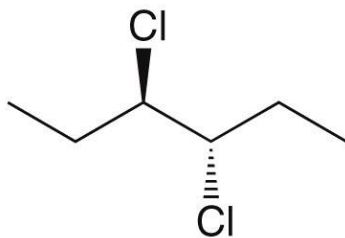
- Like Lewis structures, lines are drawn between atoms to show covalent bonds:



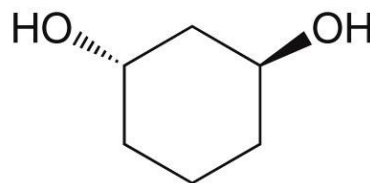
- Atoms are bonded at angles (zigzag) that represent
- Carbon atoms are not labeled, but a carbon is

3D Bond-line Structures

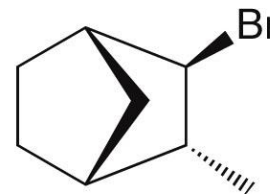
- ◆ The vast majority of molecules are 3-dimensional (3D), but it is difficult to represent a 3D molecule on a 2-dimensional (2D) piece of paper or blackboard.



Acyclic
(No ring)



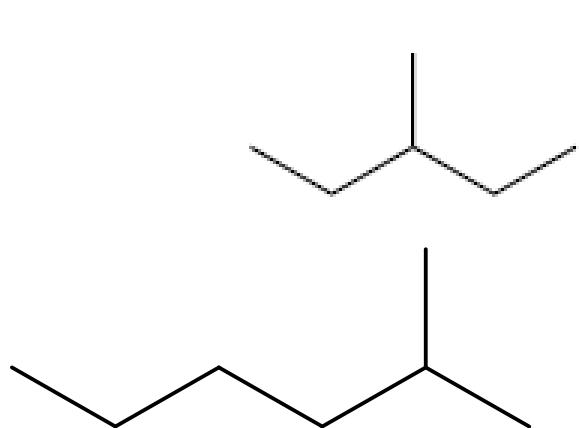
Cyclic
(One ring)



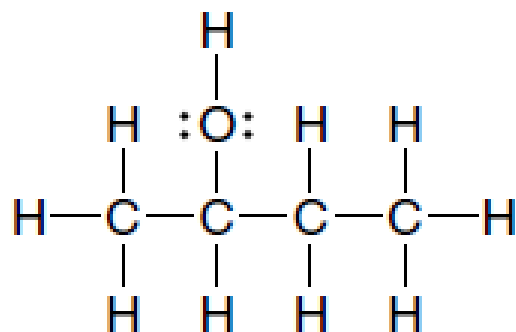
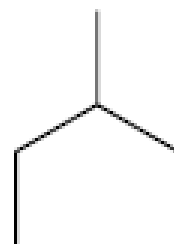
Bicyclic
(Two rings)

- ◆ *We'll come back to this when we get to Chapter 5.*

Bond-line Structures

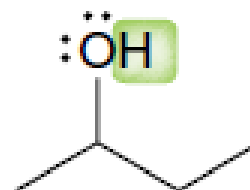


is the same as



This H must be drawn:

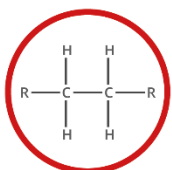
is drawn like this:



FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

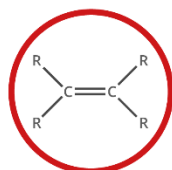
FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE BELOW, 'R' REPRESENTS A HYDROCARBON GROUP OR HYDROGEN, AND 'X' REPRESENTS ANY HALOGEN ATOM.

● HYDROCARBONS
 ● SIMPLE OXYGEN HETEROATOMICS
 ● HALOGEN HETEROATOMICS
 ● CARBONYL COMPOUNDS
 ● NITROGEN BASED
 ● SULFUR BASED
 ● AROMATIC



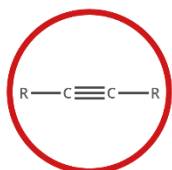
ALKANE

Naming: -ane
e.g. ethane



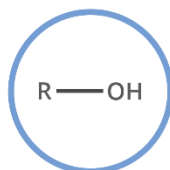
ALKENE

Naming: -ene
e.g. ethene



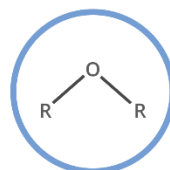
ALKYNE

Naming: -yne
e.g. ethyne



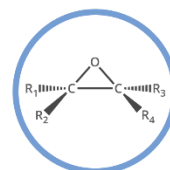
ALCOHOL

Naming: -ol
e.g. ethanol



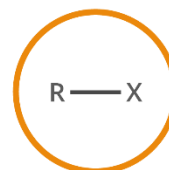
ETHER

Naming: -oxy -ane
e.g. methoxyethane



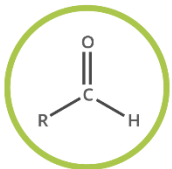
EPOXIDE

Naming: -ene oxide
e.g. ethene oxide



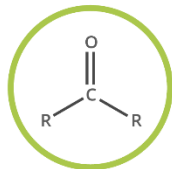
HALOALKANE

Naming: halo-
e.g. chloroethane



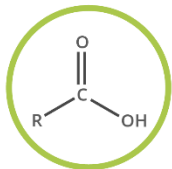
ALDEHYDE

Naming: -al
e.g. ethanal



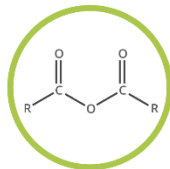
KETONE

Naming: -one
e.g. propanone



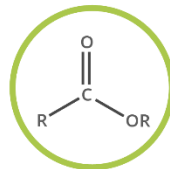
CARBOXYLIC ACID

Naming: -oic acid
e.g. ethanoic acid



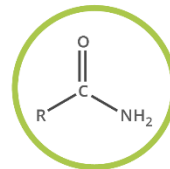
ACID ANHYDRIDE

Naming: -oic anhydride
e.g. ethanoic anhydride



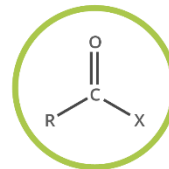
ESTER

Naming: -yl -oate
e.g. ethyl ethanoate



AMIDE

Naming: -amide
e.g. ethanamide



ACYL HALIDE

Naming: -oyl halide
e.g. ethanoyl chloride



AMINE

Naming: -amine
e.g. ethanamine



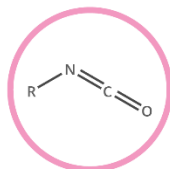
NITRILE

Naming: -nitrile
e.g. ethanenitrile



IMINE

Naming: -imine
e.g. ethanimine



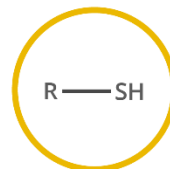
ISOCYANATE

Naming: -yl isocyanate
e.g. ethyl isocyanate



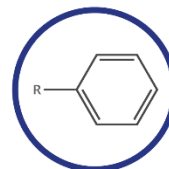
AZO COMPOUND

Naming: -azo-
e.g. azoethane



THIOL

Naming: -thiol
e.g. methanethiol



ARENE

Naming: -yl benzene
e.g. ethyl benzene



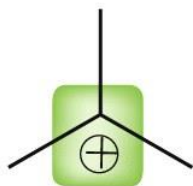
Additional Practice Problems

◆ Draw the bond-line structures from the following formulas:



Formal Charges

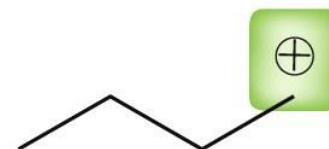
- Most carbon atoms will have FOUR covalent bonds and no lone pairs to avoid carrying a formal charge.



No hydrogen atoms
on this C⁺



One hydrogen
atom on this C⁺



Two hydrogen
atoms on this C⁺

For Next Time....

- ▶ Wednesday Chapter 2 Sections 2.7-2.11
- ▶ Homework Practice Problems Chapter 1
#8,12,15,37,39,43,45,48,49,53,56
- ▶ Homework Practice Problems Chapter 2
#1,5,12,16,25,34,40,47,48,54,55,64, 66
*know the functional groups in table 2.1