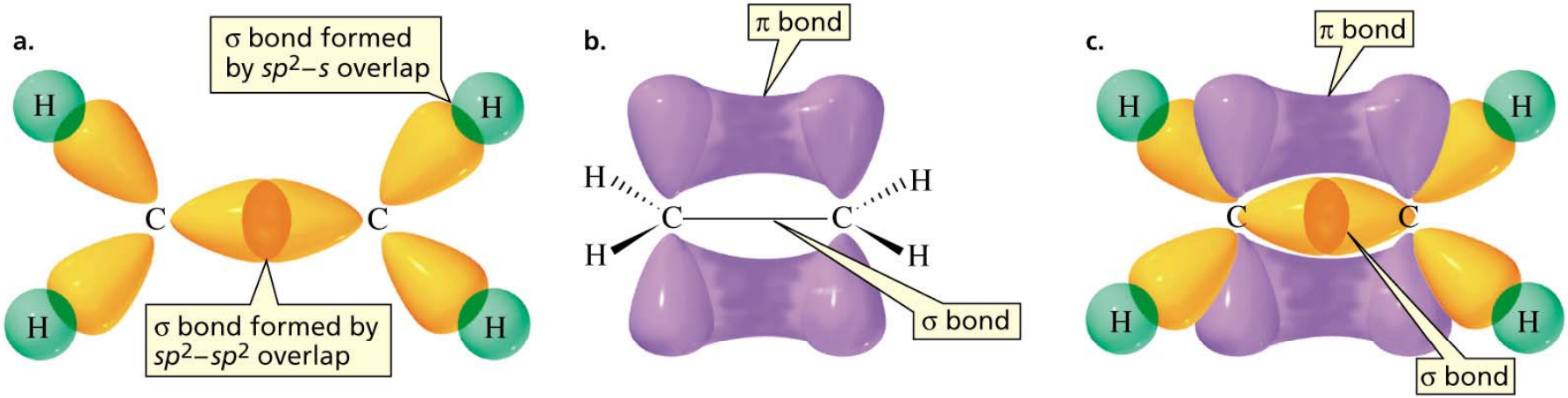
Chapter 1:
Electronic Structure and Bonding
Or
A Brief Review of General Chemistry

Part 2: Quantum Mechanics and Molecular Orbital Theory

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

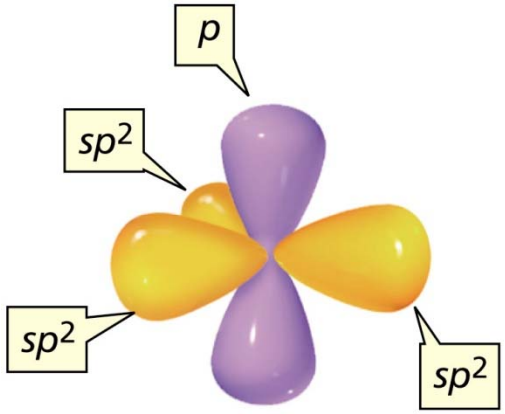
Hybrid Orbitals of Ethene, C_2H_4



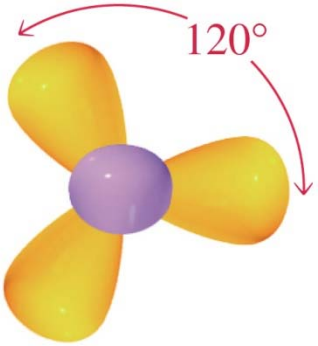
Bonding in Ethene (Ethylene): A Double Bond

- The sigma bond is unaffected by rotation of one of the CH_2 groups.
- The overlap of the p orbitals is disrupted by rotation of one of the CH_2 groups.
- This would cause the double bond to break.

Hybrid Orbitals of Ethene, C_2H_4



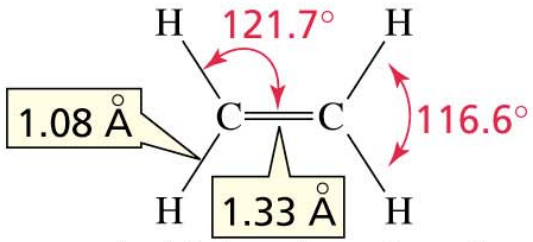
side view



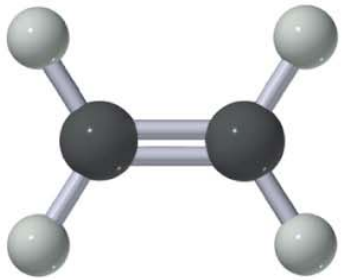
top view

An *sp*²-Hybridized Carbon -

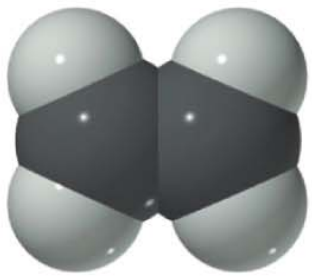
- The bond angle in the *sp*² carbon is 120°.
- The *sp*² carbon is the trigonal planar carbon.



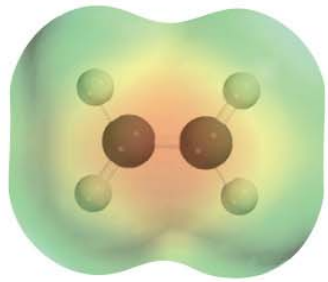
a double bond consists of one σ bond and one π bond



ball-and-stick model of ethene



space-filling model of ethene



electrostatic potential map for ethene

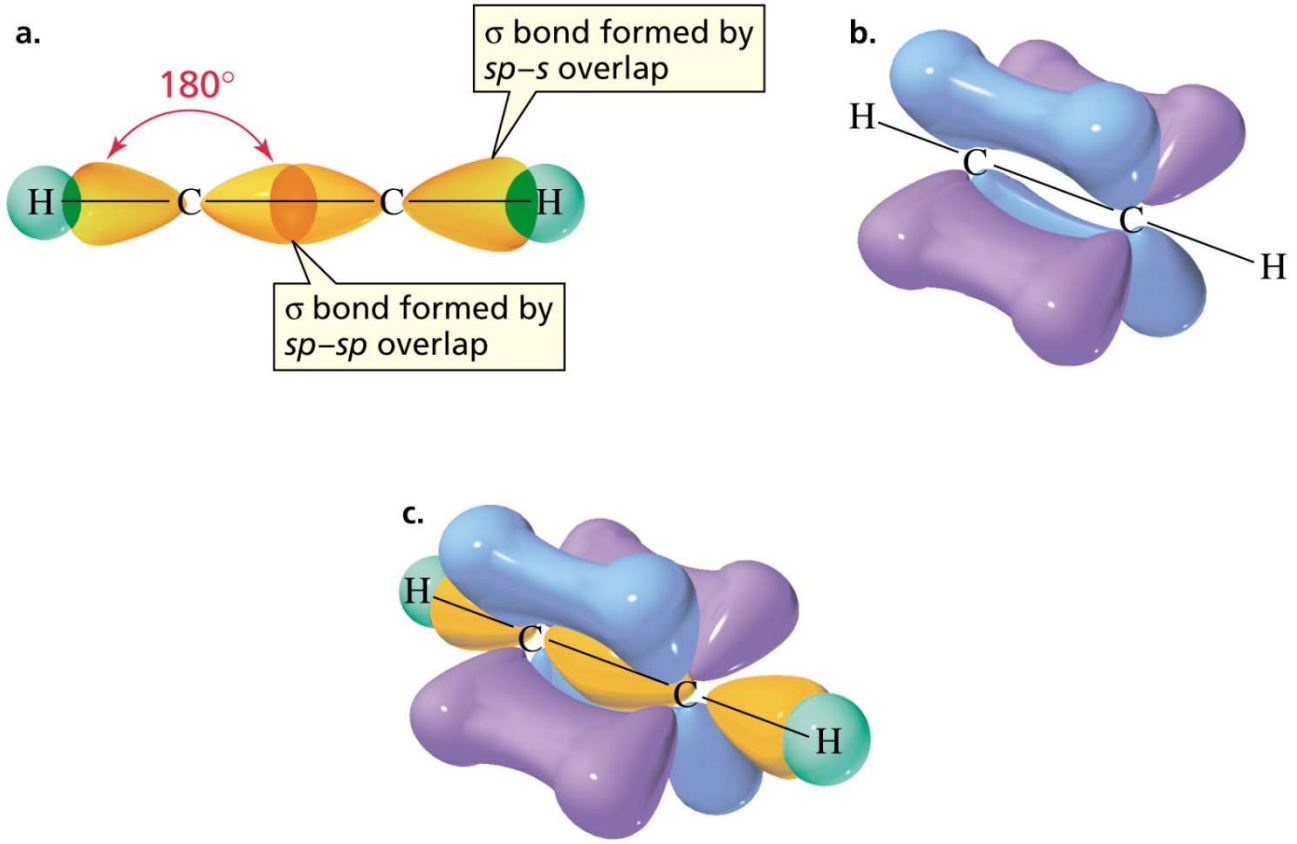
Molecular Orbital Theory

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

CHCH

Draw a Lewis Dot Structure for Ethyne

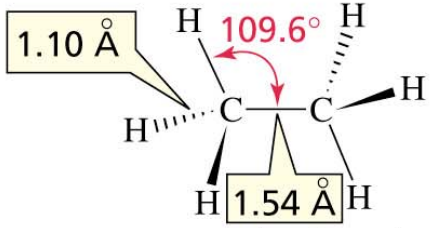
Hybrid Orbitals of Ethyne, C_2H_2



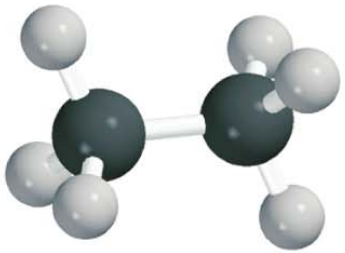
Bonding in Ethyne (Acetylene) : A Triple Bond

- A triple bond consists of one s bond and two p bonds.
- Bond angle of the *sp* carbon: 180°.

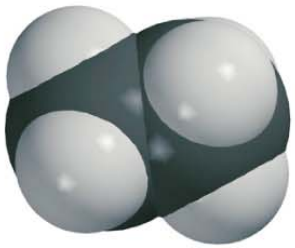
Molecular Orbital Theory



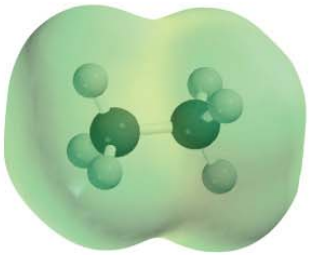
perspective formula of ethane



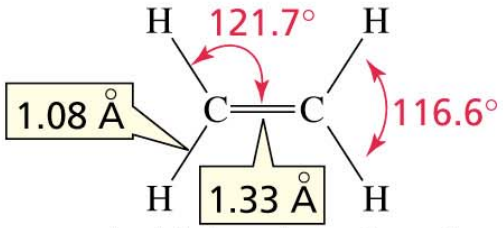
ball-and-stick model of ethane



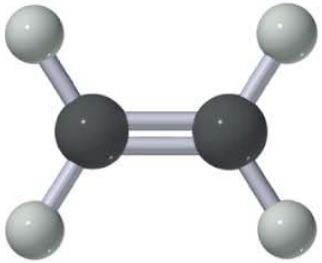
space-filling model of ethane



electrostatic potential map for ethane

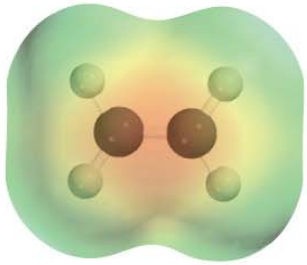


a double bond consists of one σ bond and one π bond

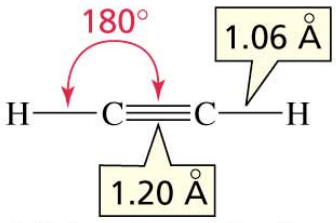


ball-and-stick model of ethene

space-filling model of ethene



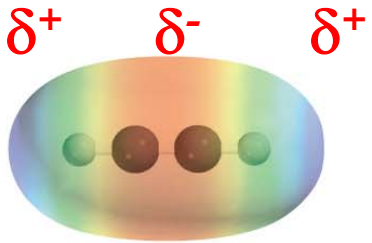
electrostatic potential map for ethene



a triple bond consists of one σ bond and two π bonds

ball-and-stick model of ethyne

space-filling model of ethyne



electrostatic potential map for ethyne

Molecular Orbital Theory

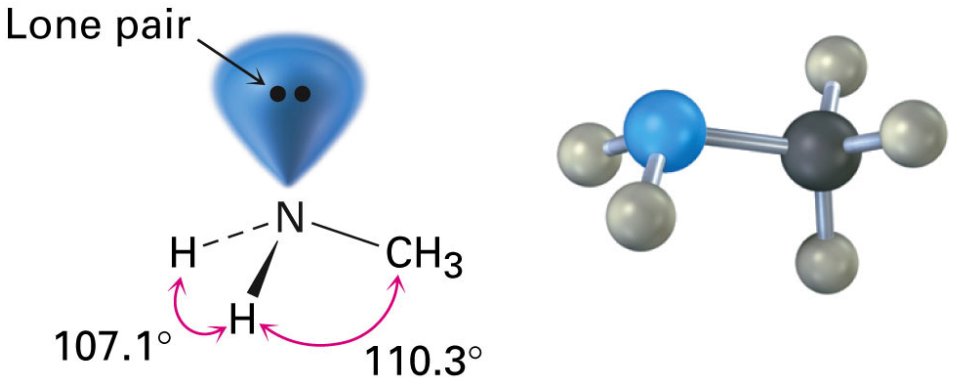
Summary

- 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.
- The greater the electron density in the region of orbital overlap, the stronger the bond.
- The more *s* character, the shorter and stronger is the bond.
- The more *s* character, the larger is the bond angle.
- A π bond is weaker than a σ bond.

Hybridization of Nitrogen and Oxygen

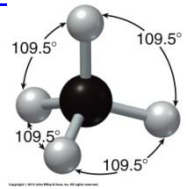
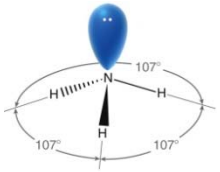
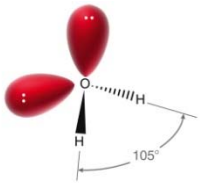
Elements other than C can have hybridized orbitals

- H–N–H bond angle in ammonia (NH_3) 107.3°
- C-N-H bond angle is 110.3 °
- N's orbitals (sppp) hybridize to form four sp^3 orbitals
- One sp^3 orbital is occupied by two nonbonding electrons, and three sp^3 orbitals have one electron each, forming bonds to H and CH_3.



Methylamine

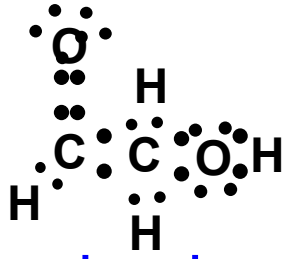
Molecular Geometry – sp^3 Geometry

Example	Steric number	Hybridization	Arrangement of electron pairs	Arrangement of atoms (geometry)
CH_4 	4	sp^3	Tetrahedral	Tetrahedral
NH_3 	4	sp3	Tetrahedral	Trigonal pyramidal
H_2O 	4	sp^3	Tetrahedral	Bent

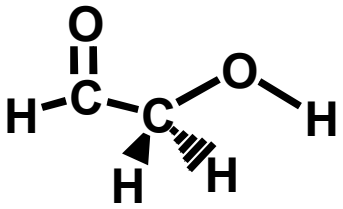
Representing Molecules

Bonding Models ($C_2H_4O_2$)

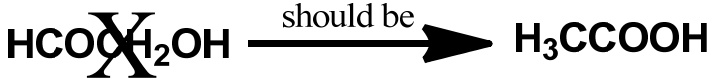
- Lewis Dot structures



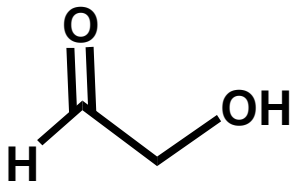
- Line structures



- Condensed structures



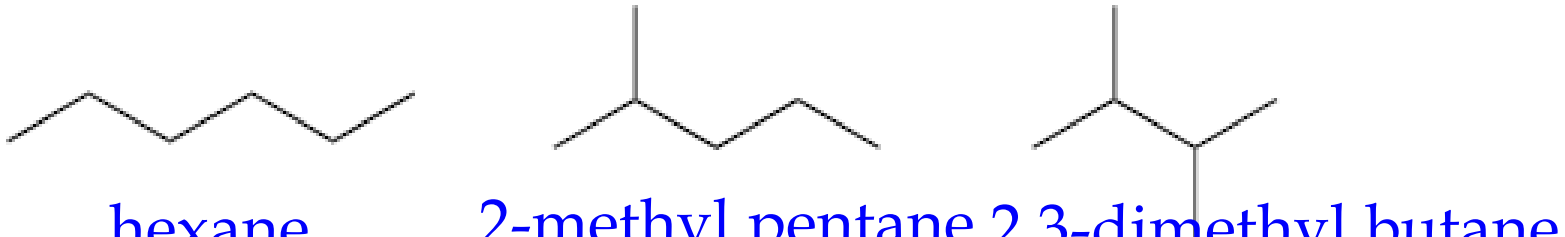
- Organic structures



- There are many ways to represent molecules.
- If you were representing a large molecule with 20 or more atoms, which structure would be most time consuming to draw?
- Which structures give you the most information about the structure?

Bond-line Structures

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

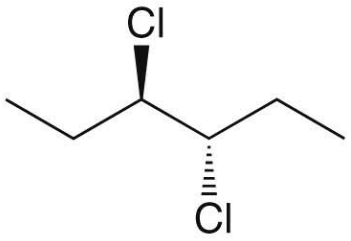


hexane 2-methyl pentane 2,3-dimethyl butane

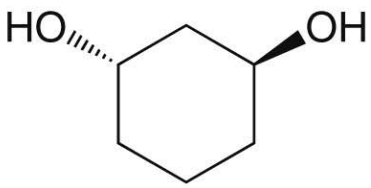
- Atoms are bonded at angles (zigzag) that represent the actual geometry of the bond angles.
- Carbon atoms are not labeled, but a carbon is assumed to be located at every corner or endpoint on the zigzag.

3D Bond-line Structures

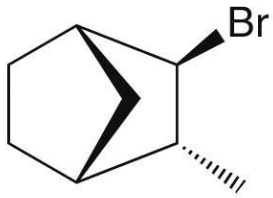
- The vast majority of molecules are 3-dimensional (3D), but it is difficult to represent a 3D molecule on a 2-dimensional (2D) piece of paper or blackboard.
- We will use **dashed** and **solid** wedges to show groups that point **back into the paper** or **out of the paper**.



Acyclic
(No ring)



Cyclic
(One ring)



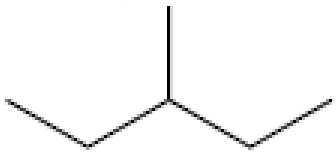
Bicyclic
(Two rings)

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

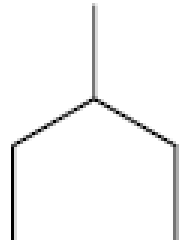
Bond-line Structures

- Single bonds are axes of rotation, so be aware that they can rotate.

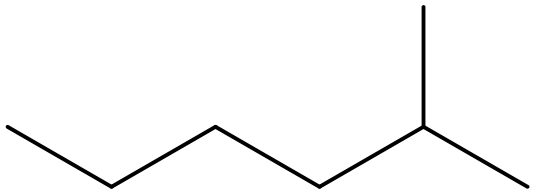
3-methyl pentane



is the same as

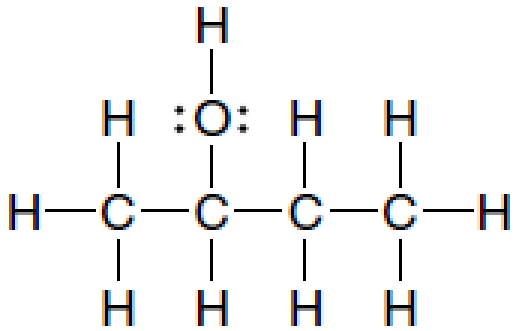


3-methyl pentane



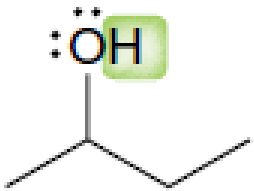
2-methyl hexane

- Heteroatoms (atoms other than C and H) should be labeled with all hydrogen atoms and lone pairs attached.



is drawn like this:

This H must be drawn:

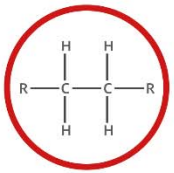


- NEVER draw a carbon with more than FOUR bonds!

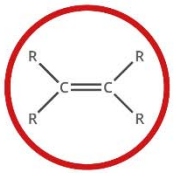
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

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.

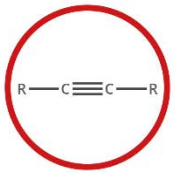
HYDROCARBONS · SIMPLE OXYGEN HETEROATOMICS · HALOGEN HETEROATOMICS · CARBONYL COMPOUNDS · NITROGEN BASED · SULFUR BASED · AROMATIC



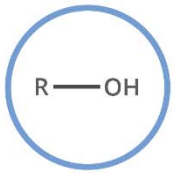
ALKANE
Naming: -ane
e.g. ethane



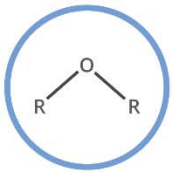
ALKENE
Naming: -ene
e.g. ethene



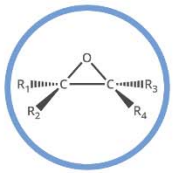
ALKYNE
Naming: -yne
e.g. ethyne



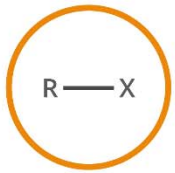
ALCOHOL
Naming: -ol
e.g. ethanol



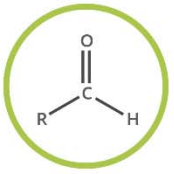
ETHER
Naming: -oxy -ane
e.g. methoxyethane



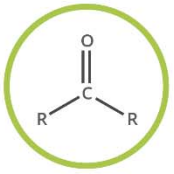
EPOXIDE
Naming: -ene oxide
e.g. ethene oxide



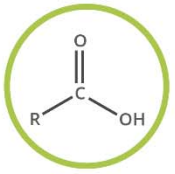
HALOALKANE
Naming: halo-
e.g. chloroethane



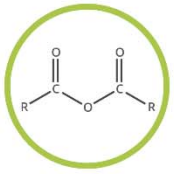
ALDEHYDE
Naming: -al
e.g. ethanal



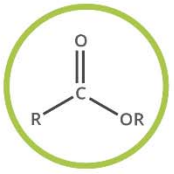
KETONE
Naming: -one
e.g. propanone



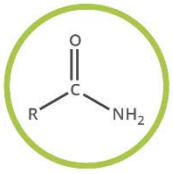
CARBOXYLIC ACID
Naming: -oic acid
e.g. ethanoic acid



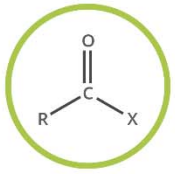
ACID ANHYDRIDE
Naming: -oic anhydride
e.g. ethanoic anhydride



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



AMIDE
Naming: -amide
e.g. ethanamide

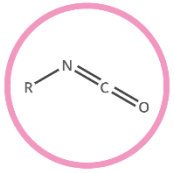


ACYL HALIDE
Naming: -oyl halide
e.g. ethanoyl chloride

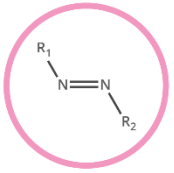
AMINE
Naming: -amine
e.g. ethanamine

NITRILE
Naming: -nitrile
e.g. ethanenitrile

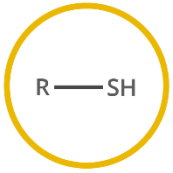
IMINE
Naming: -imine
e.g. ethanimine



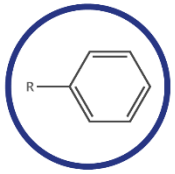
ISOCYANATE
Naming: -yl isocyanate
e.g. ethyl isocyanate



AZO COMPOUND
Naming: azo-
e.g. azoethane



THIOL
Naming: -thiol
e.g. methanethiol



ARENE
Naming: -yl benzene
e.g. ethyl benzene

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