

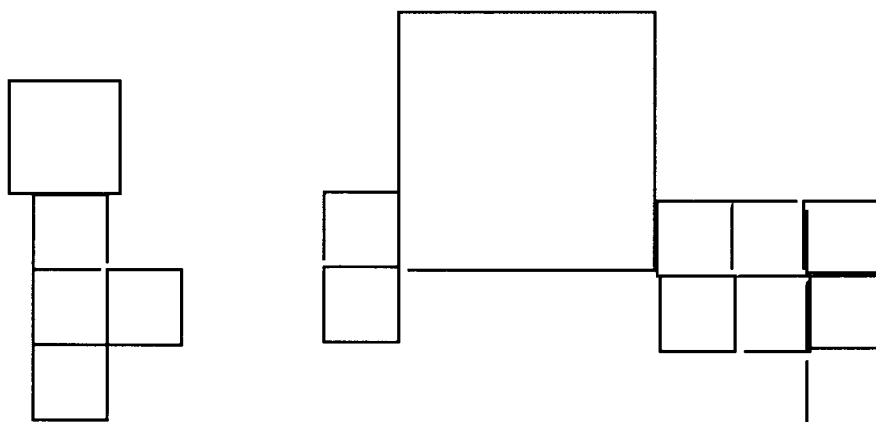
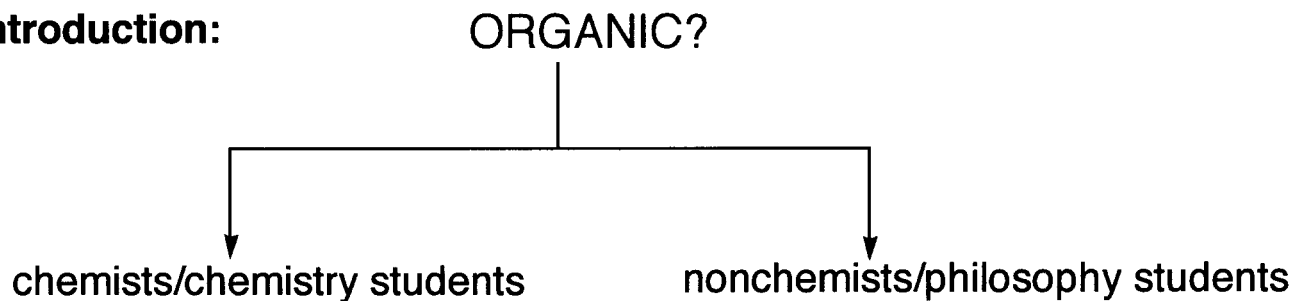
Exam 1  
Chem 3331

**Attention Students:**

The pages that follow are copies of the transparencies used in class. They are provided to make your note taking easier. You are expected to add important information and details during class. These pages do not represent a complete set of notes. You cannot survive Organic I with these notes alone!

# CHAPTER ONE: Introduction and Review

Introduction:



Review:

## I. Structure of the Atom:

A. Subatomic particles

1. electron
2. proton
3. neutron

# protons =

# protons + # neutrons =

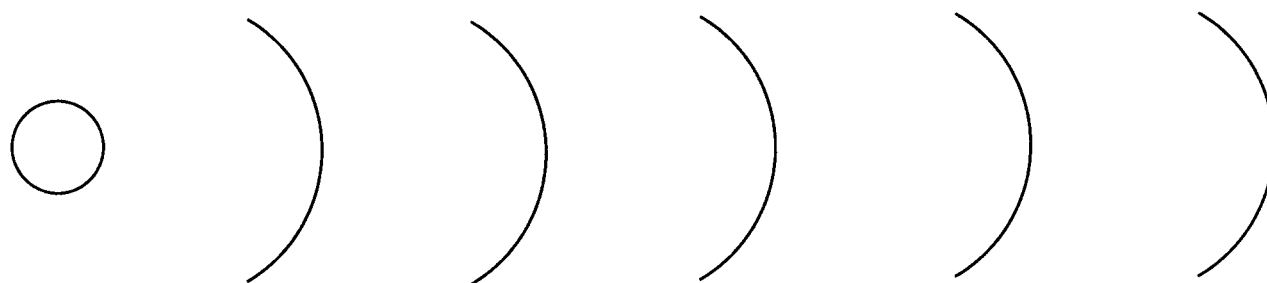
## B. Models of the Atom - where are e, P, and N?

1. Thompson
2. Rutherford
3. Bohr
4. Quantum Mechanical Model

Using a model - which one?

shells

subshells



orbitals

Orbital Shapes:



## C. Electron Configuration - distribution of electrons among an atom's orbitals

The lowest energy arrangement is called

1. Aufbau principle
2. Pauli exclusion principle
3. Hund's rule

Examples:

Nitrogen

Sodium

Why is electron configuration important to an organic chemist?

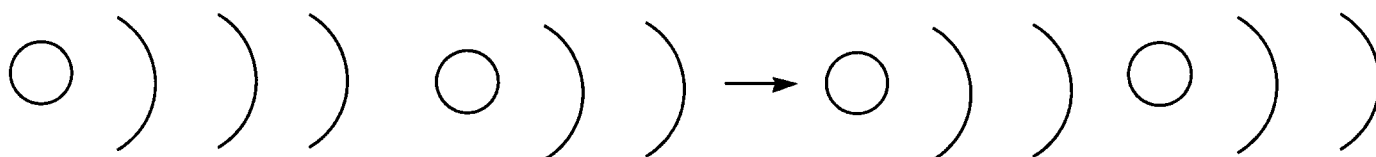
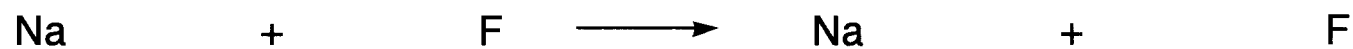
octet "rule"

How can atoms satisfy the octet rule?

## II. Bonding

### A. Ionic Bonding:

Example: NaF



### B. Covalent Bonding: The most common type of bonding in organic compounds

Simple inorganic example: H<sub>2</sub>

Representing the bonding in organic molecules will be important! (Mechanisms)

#### 1. Lewis symbol

F

O

N

C

#### 2. Lewis Structure (Electron Dot Structure)

F<sub>2</sub>

O<sub>2</sub>

N<sub>2</sub>

## TIPS FOR WRITING LEWIS STRUCTURES

1. Count the total number of valence electrons for each atom in the formula. Add or subtract electrons according to charge. The completed structure should have the same number of electrons to be correct.
  
2. Determine which atoms are bonded to which: (Hints)
  - a. H and F can only form one single bond, therefore these atoms always occupy terminal positions. (always monovalent)
  - b. Cl, Br, and I usually form single bonds in organic compounds. (usually monovalent)
  - c. S and O form single and double bonds. (usually divalent - forms 2 bonds, either 2 single or one double)
  - d. N forms single, double, and triple bonds. (usually trivalent)
  - e. C forms single, double and triple bonds and usually does not occupy a terminal position. (tetravalent with very few exceptions)
  - f. The central atom is usually the least electronegative.
  
3. Choose the central atom and draw a single bond between it and each of the surrounding atoms.

4. Complete the octets of the surrounding atoms by adding lone pairs of electrons. (except for hydrogen) Just do it!
  
5. If the octet rule is not yet satisfied for the central atom, draw double or triple bonds between it and surrounding atoms using lone pairs of electrons on appropriate atoms (atoms capable of forming double or triple bonds).
  
6. Count the valence electrons in the proposed structure. The number of electrons **MUST** match the number calculated in step one.

### C. Electronegativity and Bond Polarity

We've considered two types of bonds - ionic and covalent

transfer  $e^-$   
 ↓  
 complete transfer

share  $e^-$   
 ↓  
 equal sharing

Consider HF:

H F

electronegativity -

partial charge -

negative partial charge assigned to:

H F                      H F

rules of thumb:

smaller the difference in EN of the atoms forming a bond

greater the difference in EN of the atoms forming a bond

dipole moment -



## D. Formal Charge

The calculation of formal charge allows us to determine which atoms in a molecule bear charge - which atoms may be electron rich or electron deficient. Importance?

F.C. = # of valence electrons - # of electrons "owned" by the atom

"ownership" : all lone pairs and half of all bonding pairs

Example:  $(\text{CO}_3)^{2-}$

# valence electrons - "owned" electrons = F.C.

C

O<sub>a</sub>

O<sub>b</sub>

O<sub>c</sub>

## E. Resonance Theory

Resonance Structures:

1. Resonance structures exist only on paper! Used when a single Lewis structure is inadequate to represent the molecule. Only the hybrid exists.
2. Resonance structures differ only in the placement of electrons not atoms. "Move" only pi electrons and lone pairs.
3. All structures must be proper Lewis structures. (Atoms of periods 1 and 2 - max. of 8 electrons.)
4. All structures must have the same number of unpaired electrons (radicals).
5. Energy of the actual molecule is lower than any contributing resonance structure. (Resonance stabilization)

6. Equivalent structures make equal contributions to the resonance hybrid and will contribute to resonance stabilization.

7. Nonequivalent structures do not make equal contributions to the hybrid. The more stable the structure itself, the more it contributes to the hybrid.

8. To make decisions about the relative importance or stability of resonance contributors follow these guidelines:

a) The more covalent bonds, the more stable.

b) Structures in which all atoms have a complete octet of electrons contribute most.

c) Charge separation decreases stability. (Requires energy to separate + and - charges. ) Uncharged structures contribute more than charged structures.

d) Structures that place negative charge on the more electronegative element and positive charge on the more electropositive element are more stable and contribute more to the hybrid. (However, rule 8b is more important.)

## Structural Formulas:

A. Lewis Structure - shows all atoms, bonds, and lone pairs

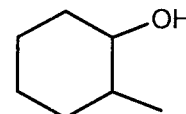
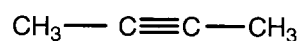
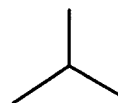
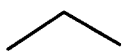
EX:  $C_3H_8O$

$C_4H_{10}O$

B. Condensed Formula - shows atoms only, not bonds  
- atoms grouped in a manner that indicates bonding in the molecule

C. Line-Angle Formula (Skeletal Formula) - carbon atoms are not drawn, and most hydrogen atoms are not drawn

1. Carbon atoms are represented by the ends and intersections of lines.
2. Each carbon is understood to have the appropriate number of hydrogens to complete the octet.  
(Hydrogen bonded to carbon is not drawn.)
3. All atoms other than carbon and hydrogen are always drawn.
4. If an atom is drawn, its hydrogen must be drawn also.



## Acids and Bases in Organic Chemistry:

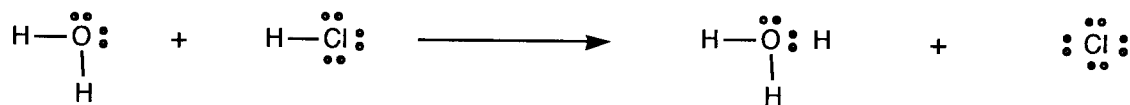
Many reactions of organic compounds may be classified as acid/base reactions. (In chapter 6, we will use the more general terms electrophile/nucleophile to describe reactions.)

### Bronsted - Lowry Acids/Bases:

acid -

base -

Example:



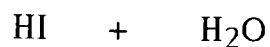
conjugate acid -

conjugate base -

acid/base pairs -

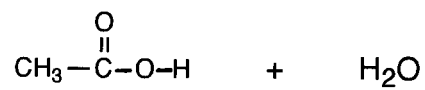
Acid/Base Strength -

Strong Acids -



stronger the acid -

Weak Acid/Base -



How Strong/Weak?

$K_a$  -  $pK_a$  -

smaller the  $pK_a$  - \_\_\_\_\_ the acid

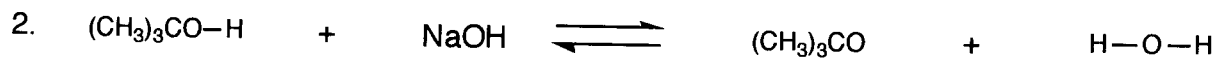
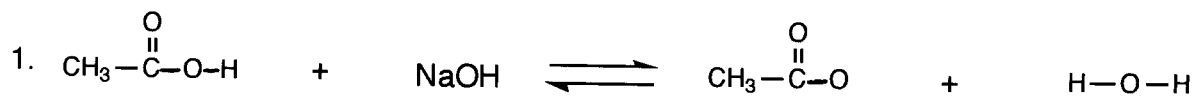
$pK_a$  of strong acids -

$pK_a$  of organic acids -

### Predicting Outcomes of Acid/Base Reactions:

Acid/Base reactions favor formation of the weaker acid and weaker base.

Examples: (use  $pK_a$ )



What if you don't have the  $pK_a$  table? Oh, no!

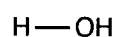
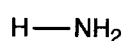
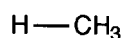
Consider the general reaction:



Factors that affect anion stability:

1. Electronegativity (EN) of the atom bearing the charge. (A more electronegative atom "tolerates" negative charge better than a less electronegative one)

compare acidities of the following:

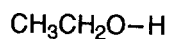


2. Delocalization of charge - the more a charge is delocalized (spread around), the more stable the system.

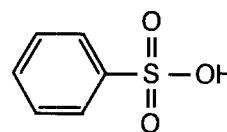
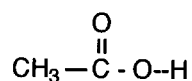
a. size of the atom - the larger the anion, the more stable the anion



b. resonance stabilization



vs



c. inductive effects (described later)

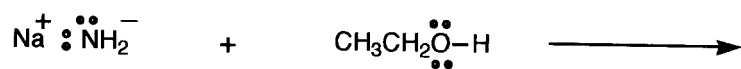
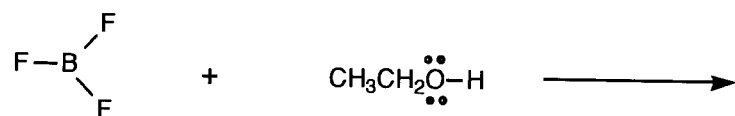
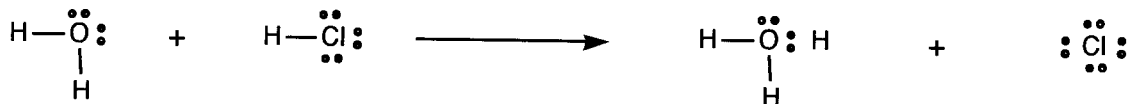


**Lewis Acids/Bases:** expands the definition of acids and bases

acid -

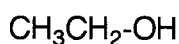
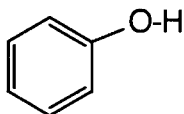
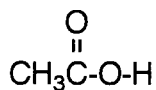
base -

includes Bronsted - Lowry acids/bases:



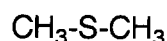
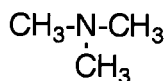
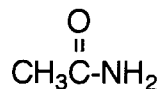
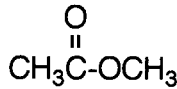
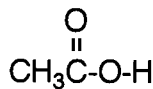
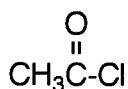
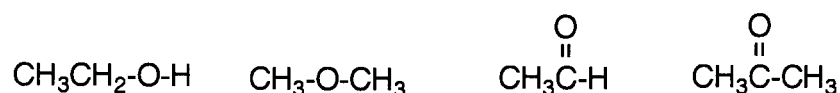
Lewis Acids\*:

H<sub>2</sub>O, HCl, HBr, HNO<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>



Li<sup>+</sup>, Mg<sup>2+</sup>, Br<sup>+</sup>

AlCl<sub>3</sub>, BF<sub>3</sub>, TiCl<sub>4</sub>, FeCl<sub>3</sub>, ZnCl<sub>2</sub>

Lewis Bases\*:

\*

**Curved Arrow Formalism: The Mechanism**

1. Curved arrows are used to indicate bonds breaking and forming in a reaction or electron "flow."
2. Direction of electron "flow" is always from electron rich to electron poor or from nucleophile to electrophile, NEVER the reverse.
3. Arrow begins with a covalent bond or a lone pair of electrons. (sometimes with a lone electron)

**REMEMBER: Arrows show where electrons flow not where the atoms go!**

See previous acid/base reactions for examples.