# Chapter 3: Polar Covalent Bonds; Acids and Bases

Concepts to Review from General Chemistry:

- ✓ Electronic Structure
- ✓ Molecular Orbitals and Atomic Orbitals
- ✓ Bonding and Antibonding
- ✓ Lewis, Condensed, or Kekule Structures
- ✓ Determining Formal Charge
- ✓ Resonance!!

Today –

- Brønstead-Lowry Acids and Bases
- Organic Acids and Bases
- Acid Dissociation Constants - pKa and pH
- Lewis Acids and Bases –
  - Nucleophiles and Electrophiles

# Acids and Bases: pH and pKa

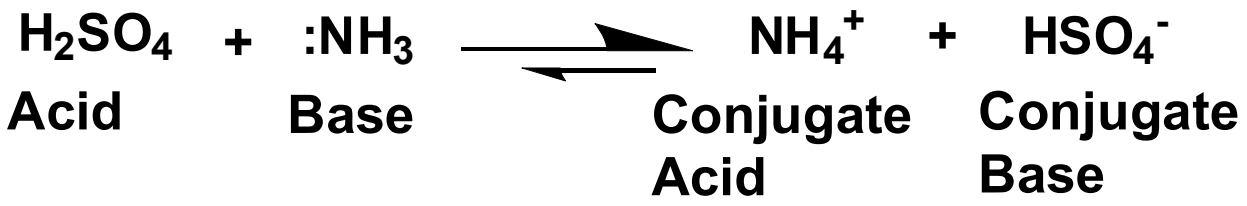
- Acid-Base reactions are some of the most common in organic chemistry.
- They are very important in biochemistry and medicine.

Remember ->

- Acidity depends on medium.
- We'll always think of $H_2O$ as standard, but often acids are less dissociated in organic solvents.

# Acids and Bases: pH and pKa

- is a species that can donate a proton.
- is a species that can accept a proton.



# Acids and Bases: pH and pKa

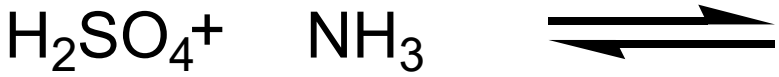
Remember from General Chemistry:

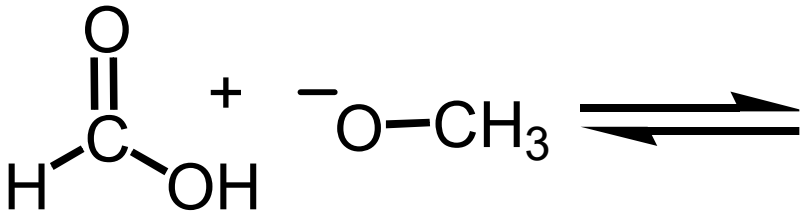
- The acidity of an aqueous solution is determined by the concentration of $H_3O^+$ ions.

- Water Autoprotolysis Constant, Kw = $1.00 \times 10^{-14}$ at $24^oC$

- In a neutral solution, $[H_3O^+]$ =

# Acids and Bases: pH and pKa

# Acids and Bases: pH and pKa

- In order to compare the reactivity of acids - what we need is a way to quantify their acid strengths.
- We can do this using the equilibrium constant for this reaction.


in $H_2O$, $[H_2O]$ = Constant, 55 Molar (M)

# Acids and Bases: pH and pKa

- $K_a$s typically range from $10^{14}$ to $10^{-50}$ in value.

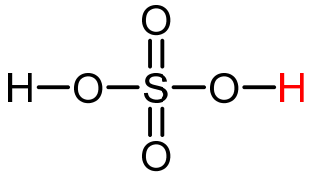
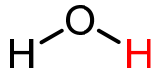
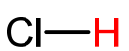
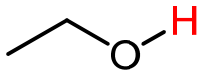
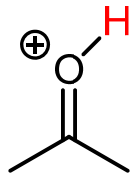
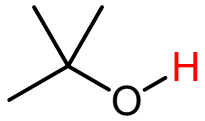
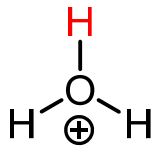
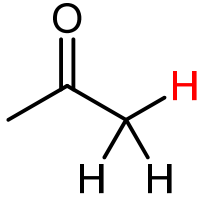
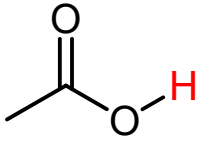
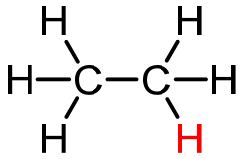
$$pK_a = -\log K_a$$

- Low or negative $pK_a$ means strong acid ➔
- High $pK_a$ value means weak acid ➔

Typical values:

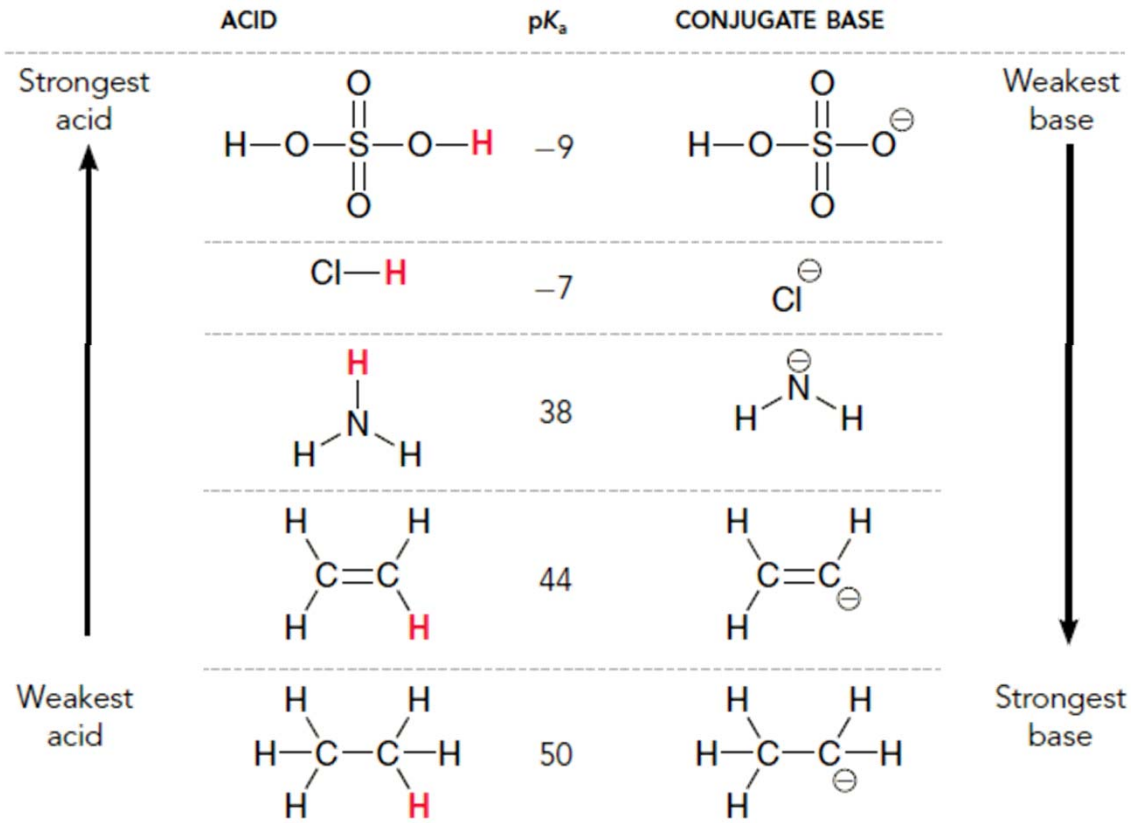
- Strong Acid
- Organic Acid
- Organic Compound

# Quantifying Acidity and Basicity – Acidity

| ACID | $pK_a$ | ACID | $pK_a$ |
|---|---|---|---|
|  | –9 |  | 15.7 |
|  | –7 |  | 16 |
|  | –2.9 |  | 18 |
|  | –1.74 |  | 19.2 |
|  | 4.75 |  | 50 |

- There are more acids and $pK_a$ values in Table 3.1.
- Each $pK_a$ unit represents an order of magnitude or a power of 10.
  - Which is stronger, HCl or $H_2SO_4$, and by exactly HOW MUCH?

# Quantifying Acidity and Basicity – Basicity

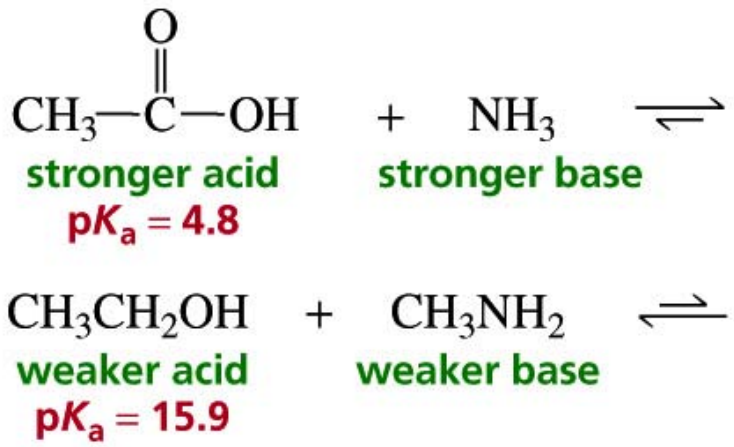



- You can also use $pK_a$ values to compare the strengths of bases:
  - The stronger the acid the weaker its conjugate base. WHY?

# Acids and Bases: pH and pKa

- Strong reacts to give weak.

- For an Acid-Base Reaction, the equilibrium lies toward the acid with the higher pKa, the predominant species at equilibrium.



# Acids and Bases: pH and pKa

The pH indicates the concentration of hydrogen ions ($H^+$)

$$pK_a = pH + \log \frac{[HA]}{[A^-]}$$

The Henderson–Hasselbalch Equation

# Acids and Bases: pH and pKa

**For a Strong Acid -**

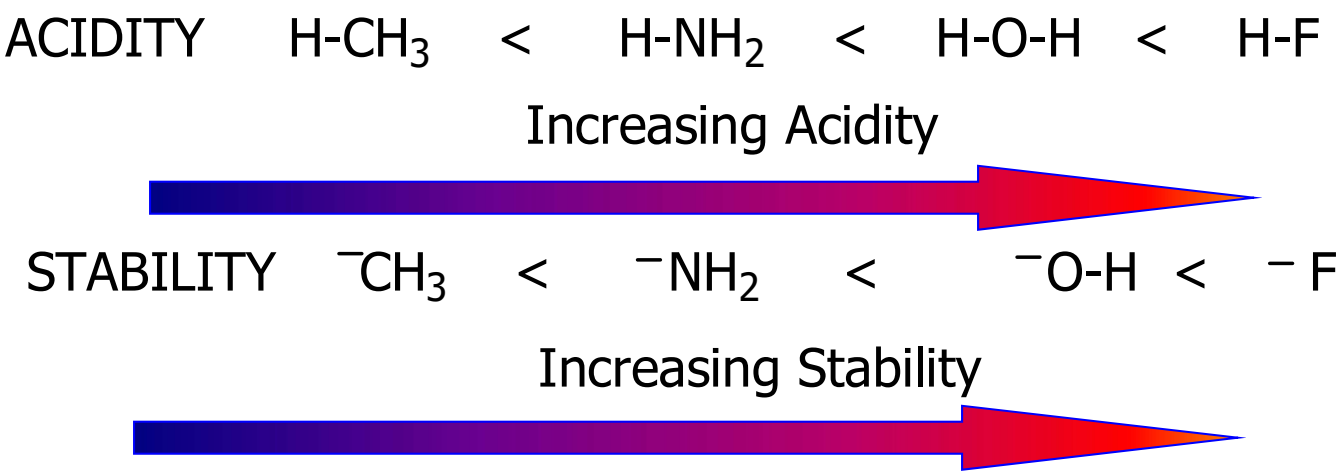
Hydrogen ion concentration, $[H^+]$, can be calculated using the following formula:

$[H^+] = 10^{-pH}$ Hydroxide ion concentration,

# Acids and Bases: pH and pKa

## Factors Influencing Acidity:

1. Electronegativity -.



# Acids and Bases: pH and pKa

## Factors Influencing Acidity:

2. Polarizability -

ACIDITY H-F < H-Cl < H-Br < H-I

Increasing Acidity

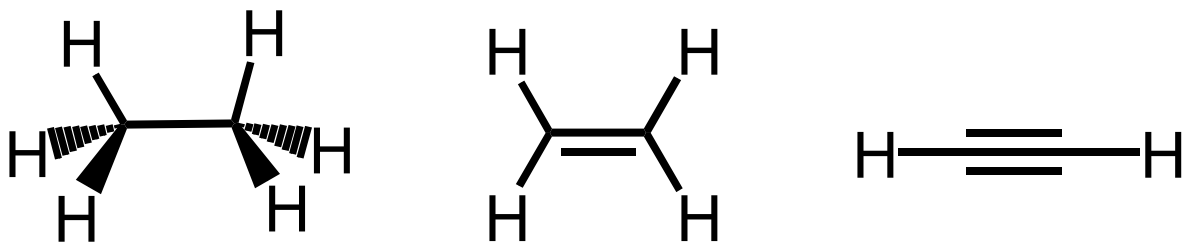
STABILITY $F^-$ < $Cl^-$ < $Br^-$ < $I^-$

Increasing Stability

# Acids and Bases: pH and pKa

## Factors Influencing Acidity:

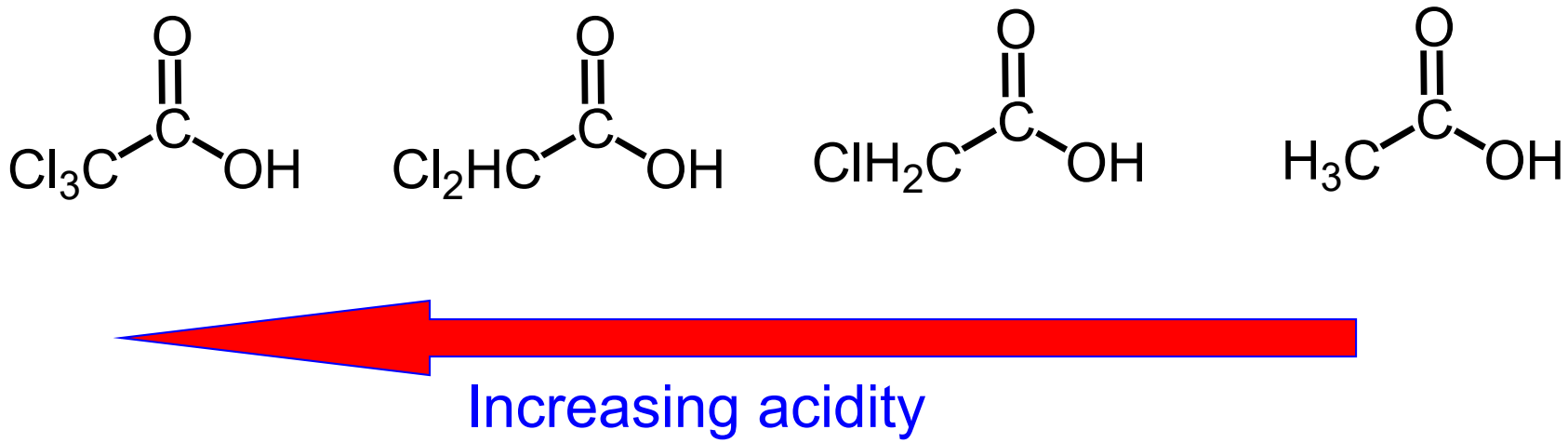
3. Hybridization -




# Acids and Bases: pH and pKa

## Factors Influencing Acidity:

4. Inductive effects –

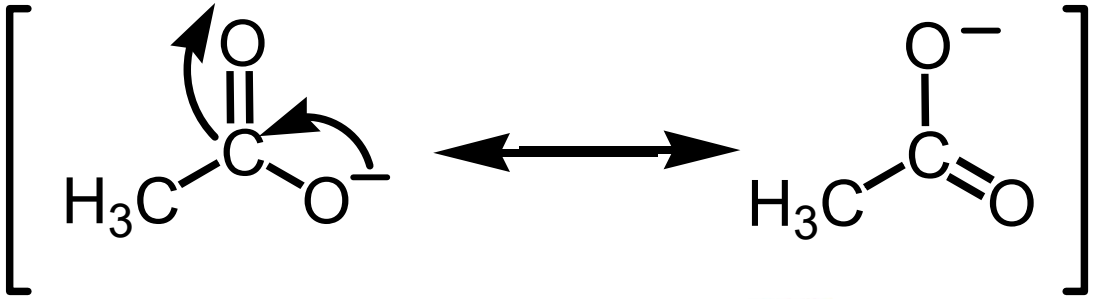


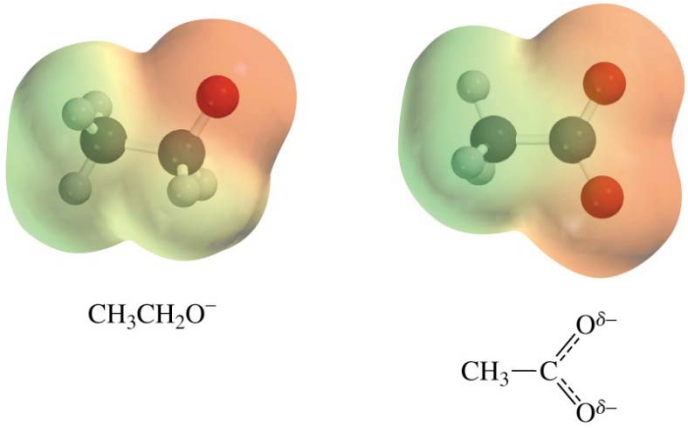
# Acids and Bases: pH and pKa

## Factors Influencing Acidity:

5. Conjugation or "Resonance"

Consider acetate anion $[CH_3COO]^-$



# Acids and Bases: pH and pKa

Factors Influencing Acidity:

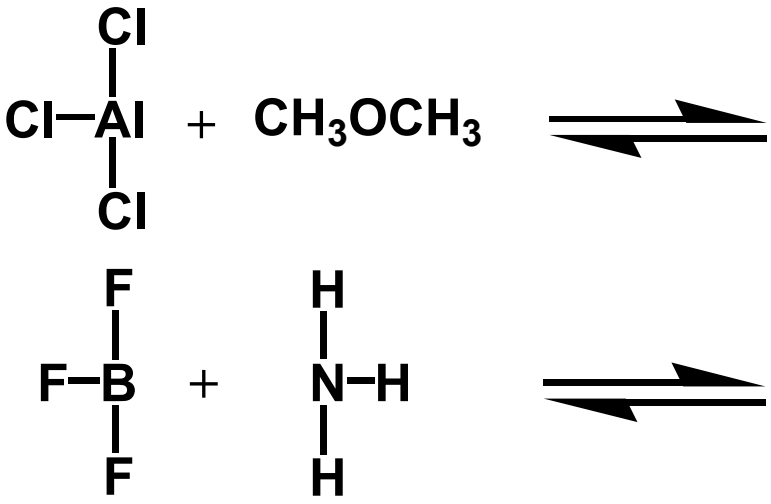
6. Stability of A- (A- = the conjugate base)

Factors that influence stability of conjugate bases (anions) are:

- Size
- Electronegativity
- Resonance

# Acids and Bases: pH and pKa

- A Lewis Acid is.
- A Lewis Base is




- Since a Lewis acid is a species that accepts electrons,

- A Lewis base is a species that donates electrons to a nucleus with an empty (or easily vacated) orbital,

# For Next Time….

- Monday is a HOLIDAY
- WEDNESDAY Finish Chapter 3 (3. 5 – 3.8)
- Friday  Start Chapter 4 (4.1 – 4.5)
  - BRING YOUR MODEL SET!

- Homework Problems Chapter 3
  #1,4,7,15,34,35,37,39,43,44, 47