(5) **Today**

Section 2.4 - 2.6: Resonance/Electron Delocalization

Section 2.7 and 2.11: Acids and Bases - Brønsted–Lowry and Lewis Definitions

Next Class (6)

Section 2.8 – 2.10: Acid and Base Strength, Acid-base Reactions, Organic Acids and Bases

Section 2.12 Noncovalent Interaction Between Molecules

(7) **Second Class from Today**

Test 1 on Chapters 1 and 2

Third Class from Today (8)

Section 3.1: Functional Groups

Section 3.2: Alkanes and Isomers

Identify ionic interactions, polar covalent bonds, and nonpolar covalent bonds ✓

Interpret electrostatic potential maps ✓

Identify polar bonds and molecules ✓

Determine the formal charge of atoms in a molecule ✓

Interpret formal charge ✓

Draw resonance contributors

Draw resonance hybrids

Weight the amount a contributor contributes to the resonance hybrid

Interpret the effects of electron delocalization

Identify Brønsted-Lowry acid and bases in acid-base reactions

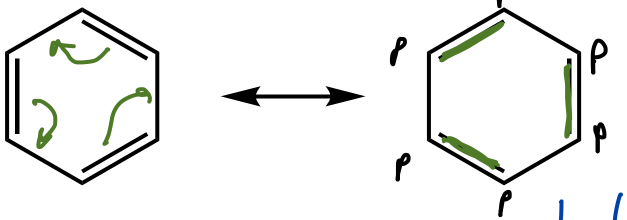
Determine acid or base strength based on pK_a

Determine or explain acid or base strength based on molecular structure

Resonance: A Way to Deal with Delocalized Electrons

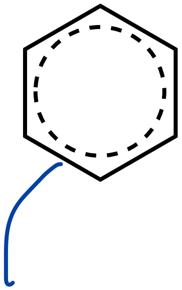
Whenever 3 or more p orbitals are in a row experiments and MO theory say that the electrons are delocalized over all of the p orbitals.

resonance contributor resonance contributor



average the resonance contributors to get the resonance hybrid

resonance hybrid



the resonance hybrid is considered the most accurate representation of the bonding that we can make while drawing skeletal structures

bond is like a 1.5 bond

more than a single bond but less than a double bond

Resonance: lone-pair electrons and resonance contributors

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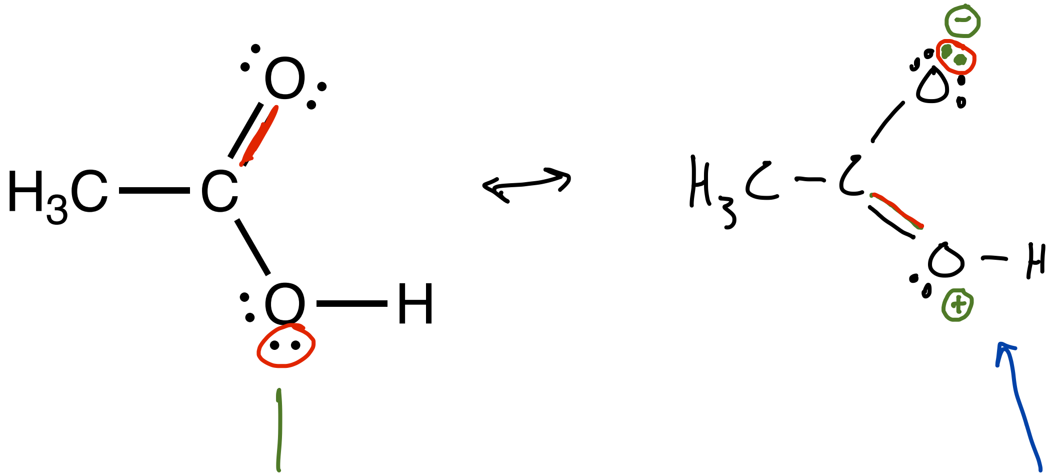


lp e⁻'s adjacent to a π bond

this is why acetic acid is an acid

Resonance: The resonance hybrid resembles...

Section 2.4 – 2.7

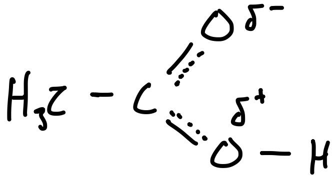
The more stable the resonance contributor is, the more it contributes to the resonance hybrid

What factors make the contributor less stable

1. Charge separation

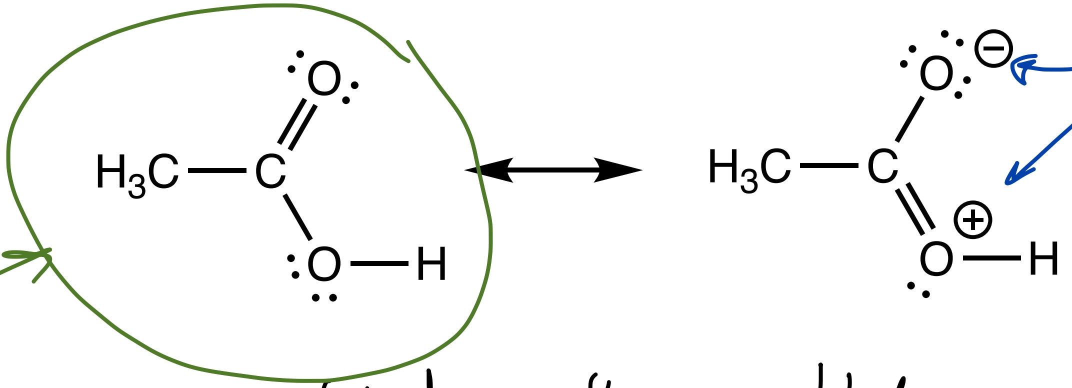
2. “Wrong” charges
    - negative charge is not on the most electronegative element and
    - a positive charge is on the most electronegative element

3. Incomplete octets



resonance hybrid

resonance hybrid more strongly resembles this contributor



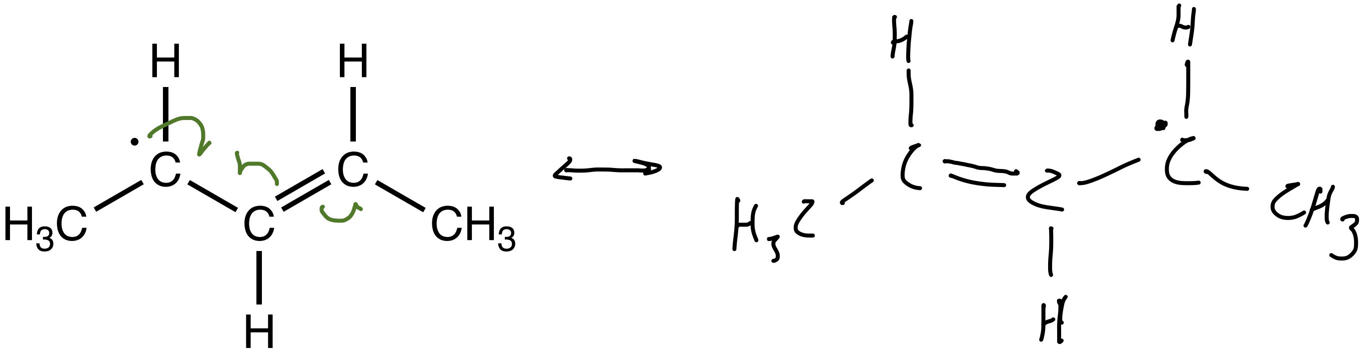
positive and negative are being held apart

resonance hybrid is the weighted average

the resonance hybrid resembles the contributor that would be lower in E

Resonance: Radical electrons

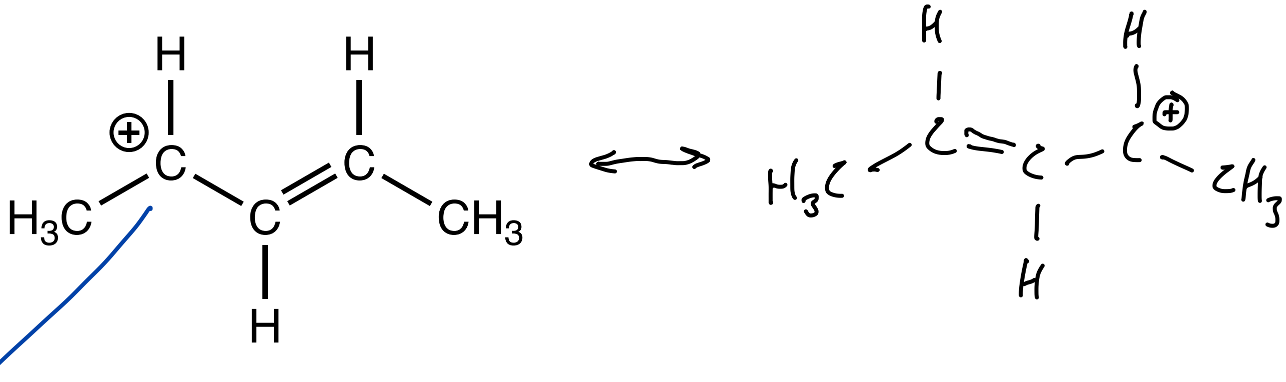
Whenever 3 or more p orbitals are in a row experiments and MO theory say that the electrons are delocalized over all of the p orbitals.



the end of the π bond
+ the unpaired e⁻
switch positions

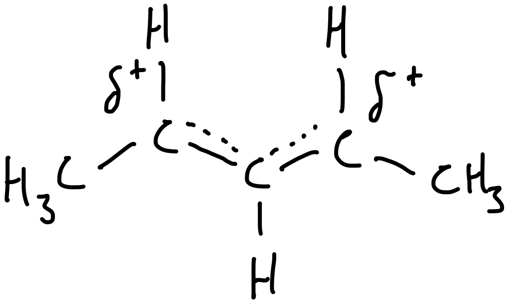
Resonance: Empty orbitals

Whenever 3 or more p orbitals are in a row, experiments and MO theory say that the electrons are delocalized over all of the p orbitals.



sp^2 hybridized
C atom
with an empty
p orbital

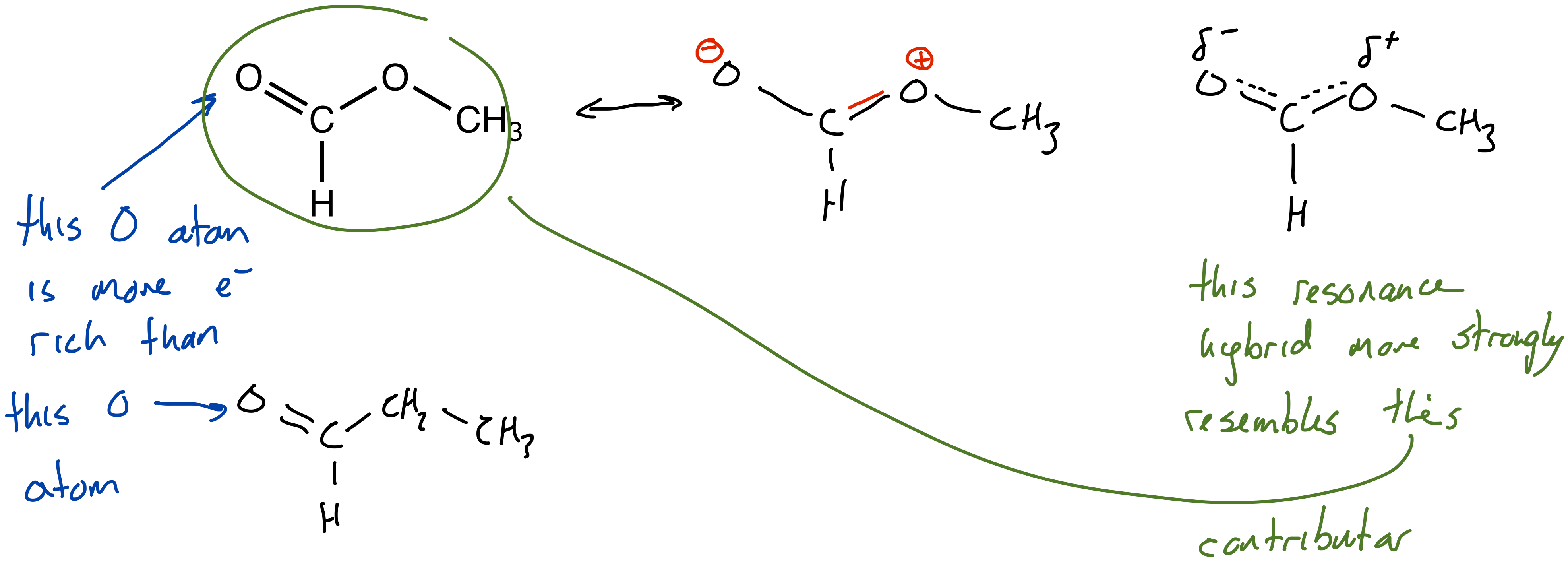
⊕ and end of
π bond are
swapped



Drawing Resonance Contributors

Rules for drawing Resonance Contributors

1. **atoms don’t move**, only electrons
2. **don’t move σ bonds**, only π bonds, lone pair e–’s, or unpaired e–’s (radicals)
3. the total number of electrons must stay the same, **don’t change the net charge**
4. p orbitals must be able to line up parallel to each other



this O atom is more e⁻ rich than this O atom

this resonance hybrid more strongly resembles this contributor

Drawing Resonance Contributors: Practice

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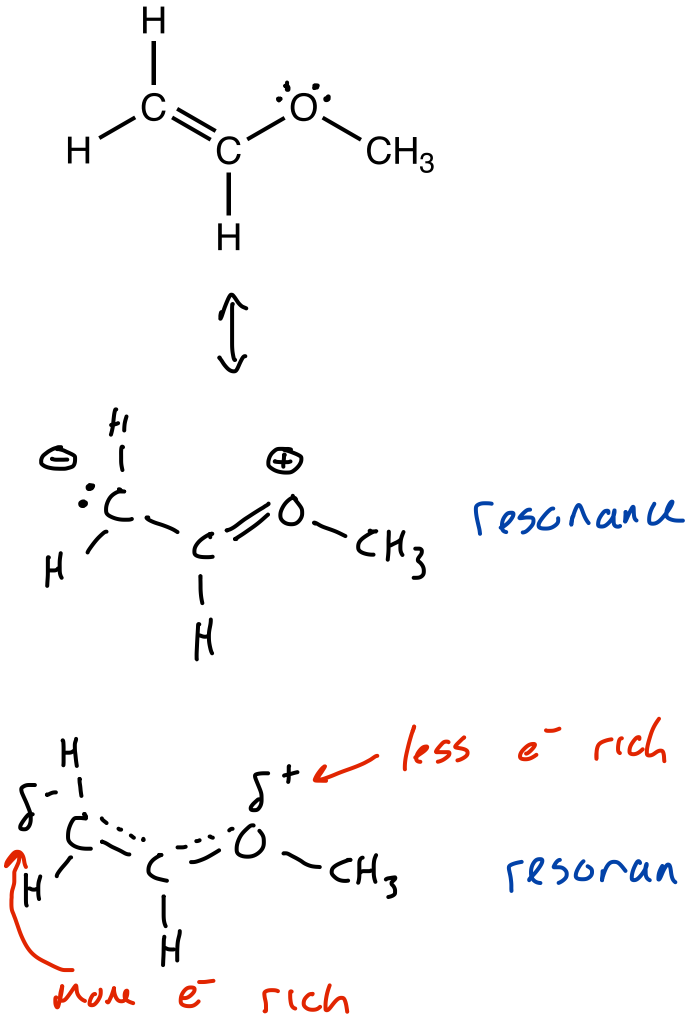
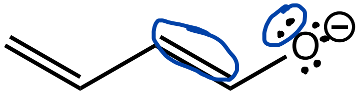
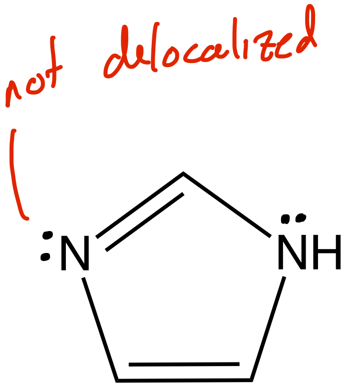


resonance contributor

resonance hybrid

2 π bonds





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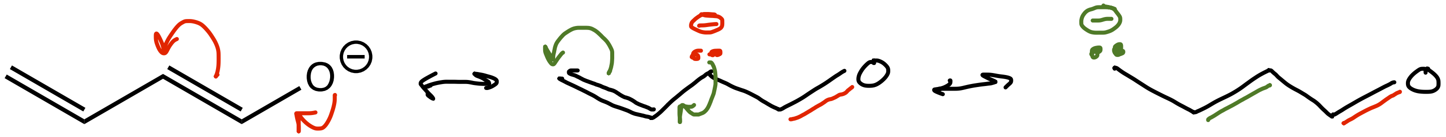
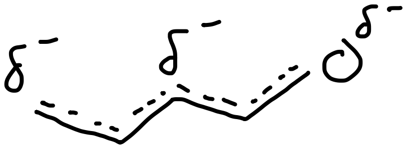
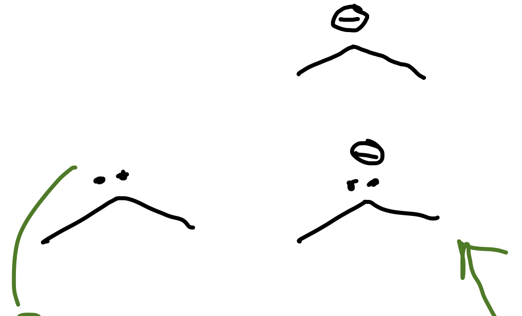




$$FC_O = -1 = 6 - (lp + 1)$$

$$6 = lp$$



If no charge is indicated this would not be the same as these

Drawing Resonance Contributors

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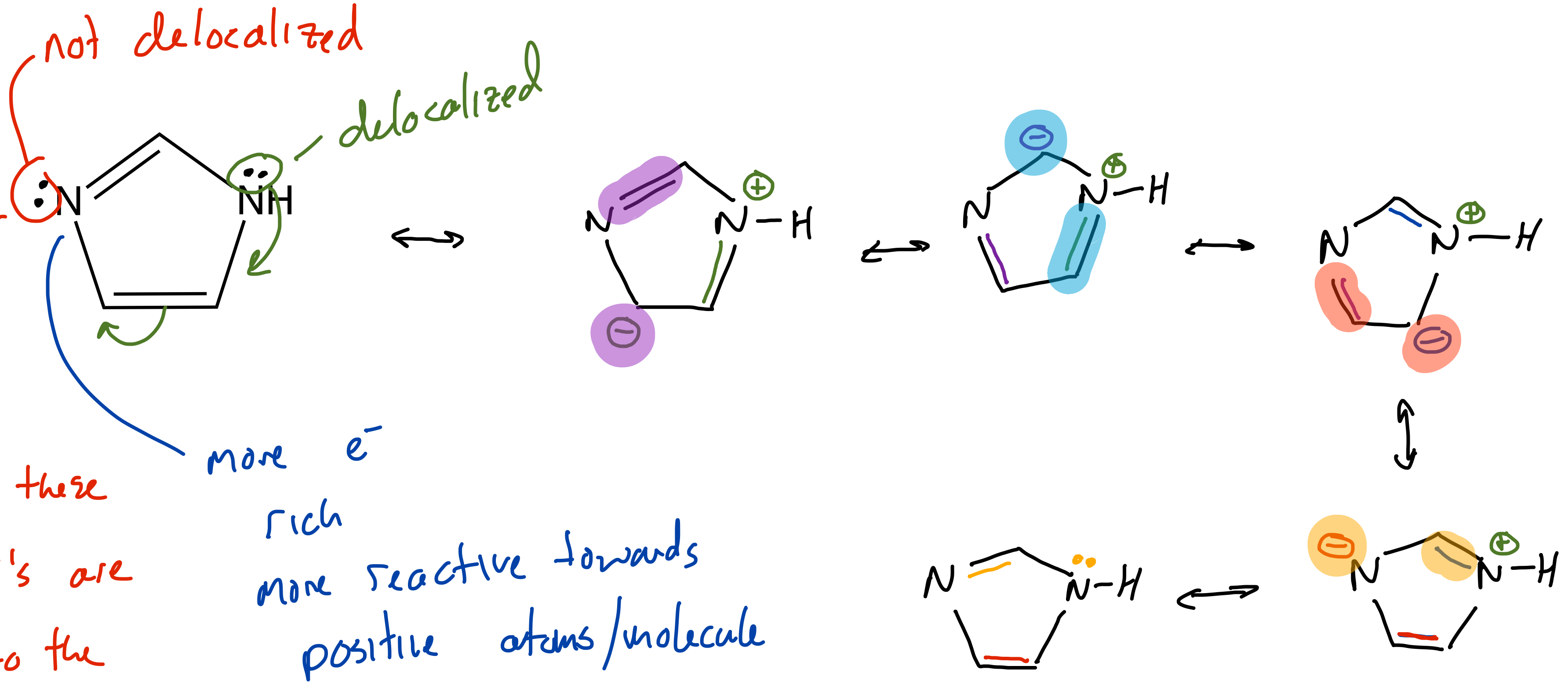


sp^2_{xy} these lp e^-'s are ⊥ to the π bond on N. The N is already using the p_z orbital to make a π bond

more e^- rich

more reactive towards positive atoms/molecule

Acids and Bases and Language

In aqueous solutions, the solution is considered **acidic** if the concentration of **H^+** is **greater than** the concentration of **OH^-**. At 25 °C, this occurs when the pH is less than 7.

In every day language, we might say that the solution is an acid. More precisely, there is a molecule **in the solution that acing as an acid and is causing the solution to be acidic**.

We will call molecules or ions **acids or bases based on how they react** (or could react).

There are **many molecules** that can **act as a base** in some circumstances **or an acid** in other circumstances.

Acids and Bases and Language

Molecules or compounds that are very likely to react as an acid are often called acids, but technically, the molecules are referred to as acids and bases based on how they react.

HNO_3, for example...

we call this nitric acid because the most likely thing for HNO_3 to do is to act like an acid

$$HNO_3 + H_2SO_4 \longrightarrow H_2NO_3^{\oplus} + HSO_4^{\ominus}$$

Brønsted-Lowry Acids and Bases

A Brønsted-Lowry acid is a proton (H^+) donors.

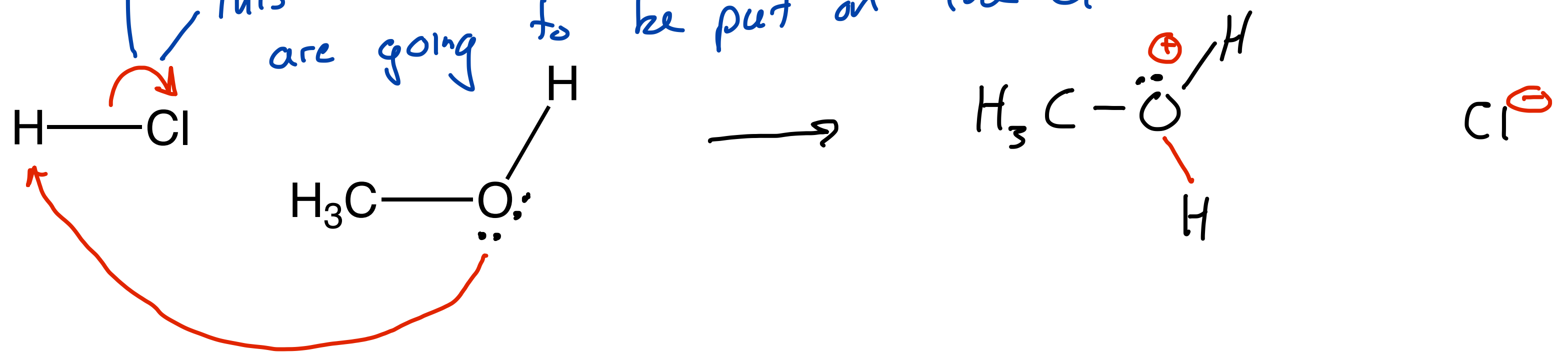
$$\underset{\text{acid}}{HCl} + \underset{\text{base}}{H_2O} \rightarrow \underset{\text{conjugate acid}}{H_3O^{\oplus}} + \underset{\text{conjugate base of HCl}}{Cl^{\ominus}}$$

A Brønsted-Lowry base is a proton (H^+) acceptor.

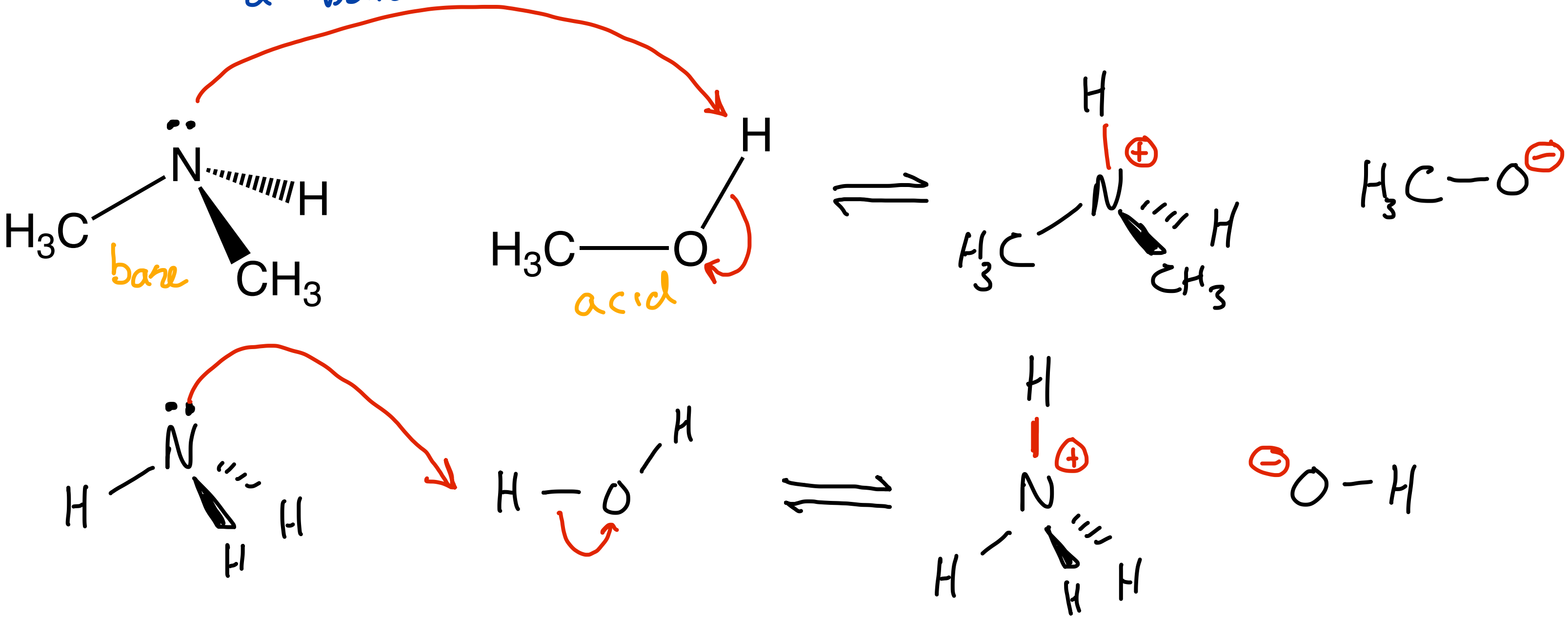
Brønsted-Lowry Acids and Bases

electron movement arrows

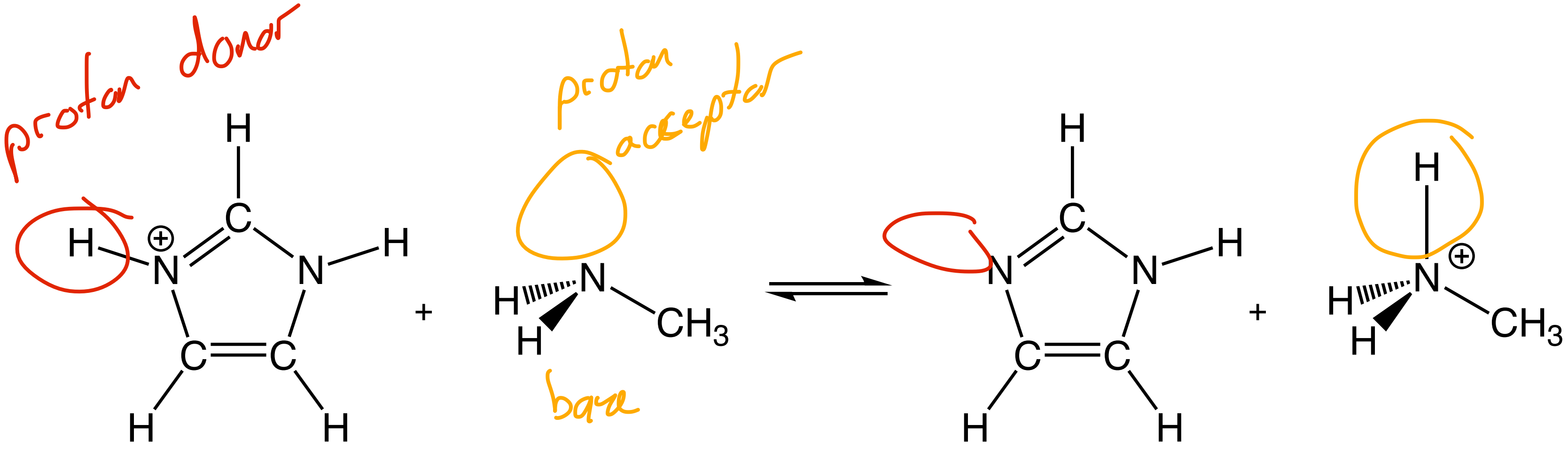
this arrow tells us that the e⁻'s in the H to Cl bond are going to be put on the Cl



this arrow tells us that these lp e⁻'s are going to make a bond to H



Brønsted-Lowry Acids and Bases



imidazole

methyl amine

K_a and pK_a

K equilibrium constant

acid ionization constant

$$HA(aq) \rightleftharpoons H^+(aq) + A^-(aq)$$

$$K_a = \frac{[H^+][A^-]}{[HA]} \qquad \frac{[prod]}{[react]}$$

large K_a means a lot of product ~~or a little bit of product~~

means large # on top small # on bottom

large K_a means strong acid

Why Tables of pKa instead of Ka?

$$pH = -\log[H^+]$$

$$pK_a = -\log K_a$$

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

buffer with a desired pH

choose an acid with pK_a close to pH because that will make a good buffer

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

choose a pH to get organic material in the form you want

charged ... more water soluble

neutral ... more organic soluble