Acids and Bases

Definitions	Acid	Base
1. Bronsted-Lowry	H+ donor	H+ acceptor
2. Lewis	e- acceptor	e- donor

Typical Acid/Base Reaction:

$$\underset{\text{Acid}}{H\text{-}A} + \underset{\text{Base}}{H_2O} \rightleftharpoons \underset{\text{Conj. acid}}{H_3O^{\oplus}} + \underset{\text{Conj. base}}{A^{\ominus}}$$

Keq for this example: / **Ka for this example:**

$$Keq = \frac{[H_3O^{\oplus}][A^{\ominus}]}{[H_2O][HA]} \qquad Ka = \frac{[H_3O^{\oplus}][A^{\ominus}]}{[HA]}$$

In general:

- Strong acid → Weak conj. base
- Weak acid → Strong conj. base
- Strong base → Weak conj. acid
- Weak base → Strong conj.acid

Predicting equilibrium:

Start by labeling the pKas in the reaction (see list)

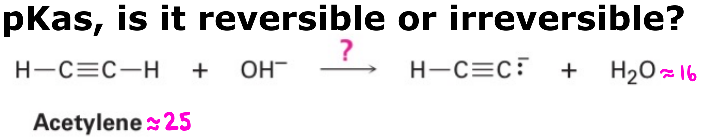
Reaction Arrows:

- RXN arrows point towards the side with the weaker acid (higher pKa)

Is it reversible or irreversible?

- Look at the difference of pKas between reactants/products
- Δ pKa >8 => irreversible rxn
- Δ pKa <8 => reversible rxn

Example: Predict equilibrium using pKas, is it reversible or irreversible?



1. Label pKas
2. Know arrows will point towards weaker acid (higher pKa), so left
3. Is it reversible or irreversible? (25-16>8), so irreversible
4. Final arrows: <—

Things to know about acid/base reactions:

Equilibrium constant (Keq): a ratio that tells the position of a chemical equilibrium

$$Keq = \frac{[products]}{[reactants]}$$

Trends:

- Keq >1 => Favors products
- Keq =1 => At equilibrium
- Keq <1 => Favors reactants (rxn doesn't work)

Acid Dissociation Constant (Ka): measure of acid strength

$$Ka = Keq\,[H_2O]$$

Trends:

↑Ka =
- Strong acid
- Full dissociation
- High [products] (large numerator)

↓Ka =
- Weak acid
- Partial/Incomplete dissociation
- High [reactants] (large denominator)

pKa =-log Ka

Trends:

↓pKa =Strong acid (↑Ka)

↑pKa = Weak acid (↓Ka)

- pKa < 1=> Strong acid
- pKa 1-3=> Moderately strong acid
- pKa 3-5=> Weak acid
- pKa >5=> Very weak acid

pKas to Know:

- sp3 C-H 51
- sp2 C-H 44
- sp C-H 25
- Water H_2O ≈16 (15.7)
- Ethanol OH ≈16 (15.9)
- Ammonia NH_3 38
- Acetic Acid CO_2H ≈5 (4.76)
- HCl -7

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How do you know which H the base will take/acid will donate?

1. **Electronegativity** (comparing atoms in the same row of periodic table)
2. **Hybridization** (% S character)
3. **Size** (comparing atoms in the same column of periodic table)
4. **Inductive effects** (happens bc of electronegative atoms elsewhere on compound)
5. **Resonance** (looking at potential products stability)

1. Electronegativity

- Atoms in same row of periodic table
- The more electronegative atom will donate H be most acidic
- **Acid strength: C < N < O < F**

2. Hybridization

- Must be comparing same atom (ex: H-C≡C-H vs. CH2=CH2 vs. CH4)
- H on atom w/ greater %S character is the stronger acid
- SP = 50% S character
- SP2 = 33% S character
- SP3 = 25% S character
- **Acid strength: sp3 < sp2 < sp**

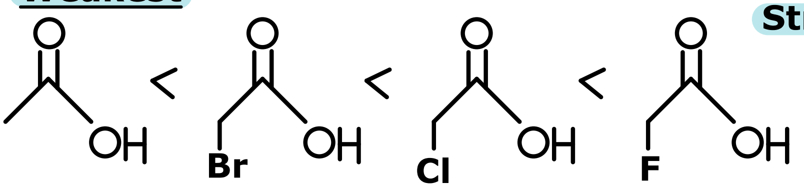
3. Size

- Atoms in same column of periodic table
- H attached to larger atom is the stronger acid
- Longer bond length = weaker bond = stronger acid
- Shorter bond length = stronger bond = weaker acid
- **Acid strength: F < Cl < Br < I**

4. Inductive effects

- Through bond effects from electronegative atoms elsewhere on compound
1. Distance matters
2. Electronegativity matters
- **Example 1: comparing different electronegative atoms in same position of carbon chain**

Weakest

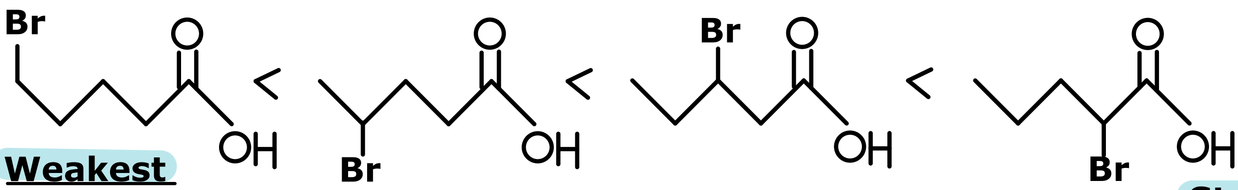


Strongest

Why?

Electronegative atoms pull electron density (via sigma bonds) towards activity site. This decreases the electron density about the oxygen, making the hydrogen easier to take off => stronger acid

- **Example 2: Same EN atom in a different location of the carbon chain**



Weakest

Strongest

Why?

The electronegative atom is pulling electron density towards it and away from what is holding onto the hydrogen. The closer the electronegative atom is to the reactive site, the stronger the pull, and the stronger the acid.

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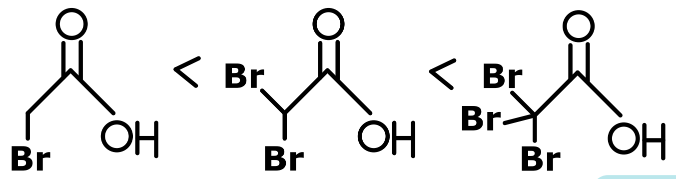
- **Example 3: Effects of multiple EN groups**



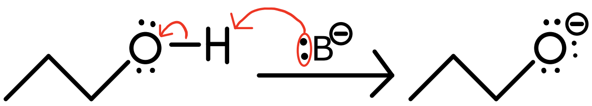
Weakest **Strongest**

Why?
The more electronegative atoms makes the acid stronger.

5. Resonance

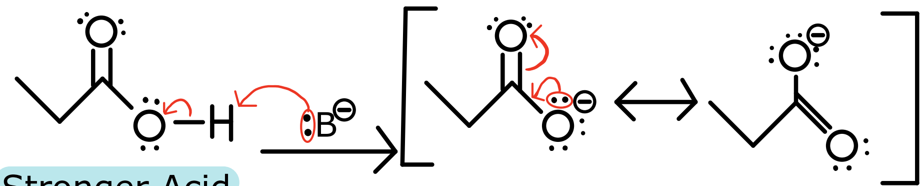
- React the acid with a generic base to generate its conjugate base
- More resonance = more stable
- If the conjugate base is stable (has more resonance), it is a weaker conjugate base, so it came from a more unstable, stronger acid
- If the conjugate base is unstable (has less resonance), it is a stronger conjugate base, so it came from a more stable, weaker acid

- **Example 1:**



Weaker acid

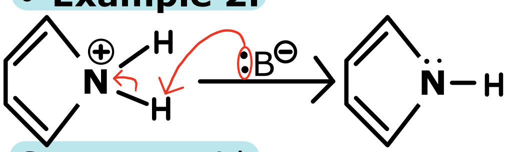
- This is the stronger conjugate base because it is more reactive and unstable, so it came from the weaker acid



Stronger Acid

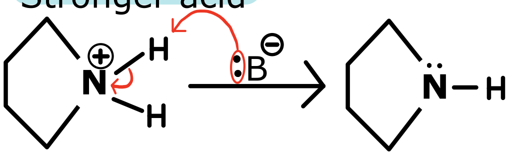
- Since there is resonance, this is the less reactive and more stable weaker conjugate base, so it came from the stronger acid

- **Example 2:**



Stronger acid

- This has 5 total resonance structures, so this conjugate base is more stable, less reactive, and weaker, so it came from the stronger acid



Weaker Acid

- This is the more unstable, stronger, more reactive conjugate base, so it came from the weaker acid