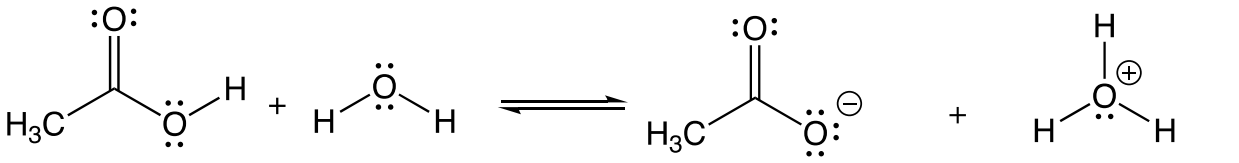


Acid (H-A) Base (B:) Conjugate Base ($A^{\ominus}$) Conjugate Acid (B-$H^{\oplus}$)

At equilibrium: $K_{equilibrium} = \frac{[Products]}{[Reactants]} = \frac{[CH_3CO_2^{\ominus}]\,[H_3O^{\oplus}]}{[CH_3CO_2H]\,[H_2O]}$

Equilibrium Constant

Assume: $[H_2O] = 55$ M and does not change

Acid Constant

$K_a = K_{equilibrium}\,[H_2O] = K_{equilibrium}\,[55\ M]$

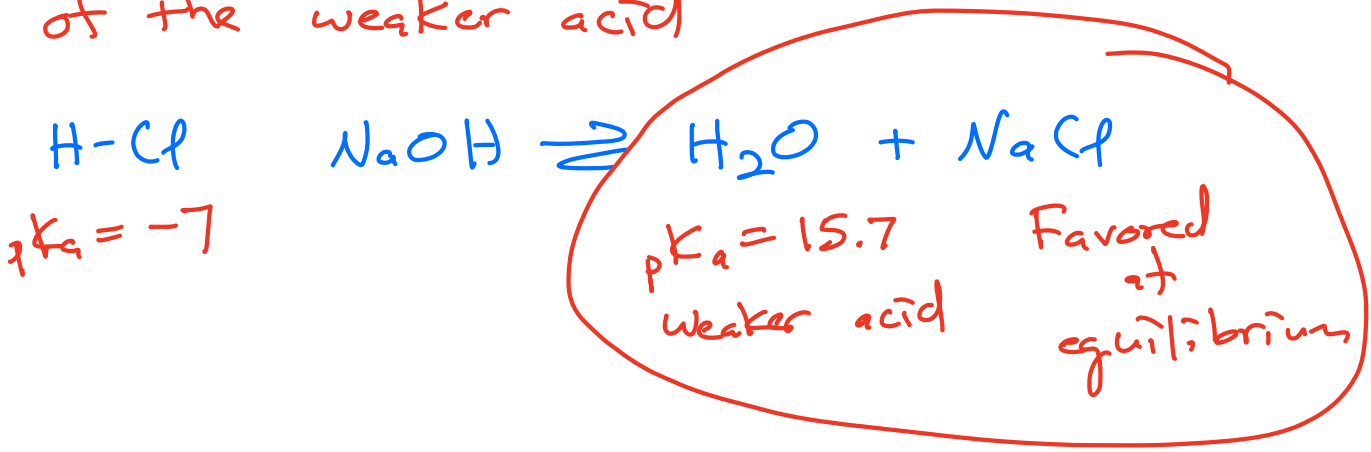
$K_a = \frac{[CH_3CO_2^{\ominus}]\,[H_3O^{\oplus}]}{[CH_3CO_2H]}$ $\qquad pK_a = -\log K_a$

A stronger acid has a lower value of pK_a

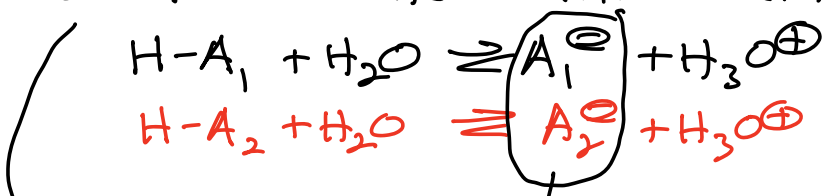
A weaker acid has a higher value of pK_a

General Rule

All acid-base reactions favor formation of the weaker acid



How to estimate relative acid strengths



Compare the relative stabilities of the anions produced upon deprotonation → the more stable anion comes from the stronger acid

How do you predict anion stability?

2 important principles for predicting anion stability

1) Negative charge (⊖) is neutralized by nuclear ⊕ charge.

2) Delocalizing negative charge (⊖) over a larger area is better. → Golden Rule #5

Rules for anion stability —

The anion is more stable when the negative charge (⊖) is:

a) On a more electronegative element (Principle 1)
→ Periodic Table (across a single row)

b) On a larger atom (Principle 2)
↓ Periodic Table (down a single column)

c) On an atom with more "s" character to its hybridization
($sp > sp^2 > sp^3$)
← anion stability

"s" orbitals are closer to the nucleus (Principle 1)

d) stabilized by resonance delocalization. (Principle 2)

e) Stabilized by the inductive effect (Principles 1 and 2)

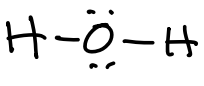
Operates through sigma bonds

nearby electronegative atoms attract ⊖ charge and therefore spread the ⊖ charge onto more atoms

Examples

Rule a)

Ex.

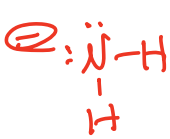


$pK_a = 15.7$

more stable anion

O is more electronegative

$pK_a = 38$

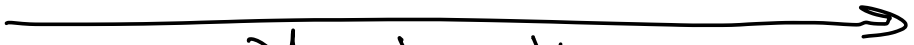


Rule b)

(Only compare ions in same column of the Periodic Table)

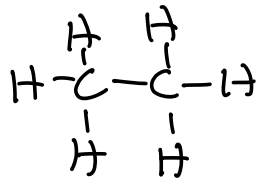
pK_a	3.5	-7	-8	-9
	H-F	H-Cl	H-Br	H-I
	$F^\ominus$	$Cl^\ominus$	$Br^\ominus$	$I^\ominus$

larger ion

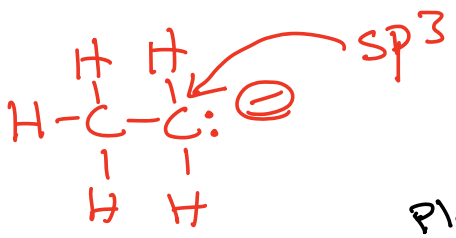


acid strength

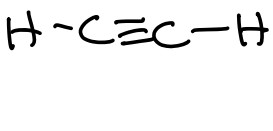
Rule c)



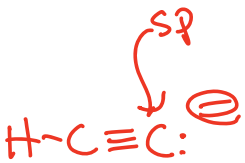
$pK_a \cong 50$



$sp^3 \rightarrow$ 25% s
75% p



$pK_a = 25$

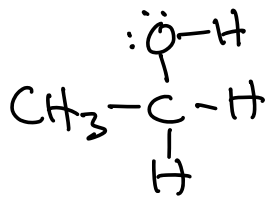


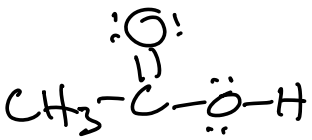
Places more ⊖ closer to nucleus

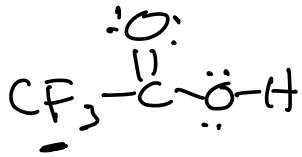
More "s" →
sp → 50% s
50% p

More stable anion

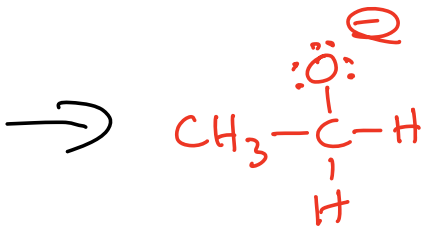
Rules d) and e)

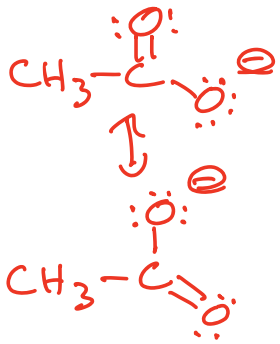


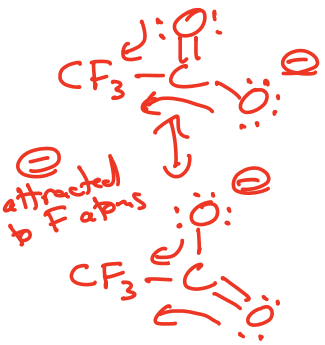




pKa 15.9 4.8 0.1





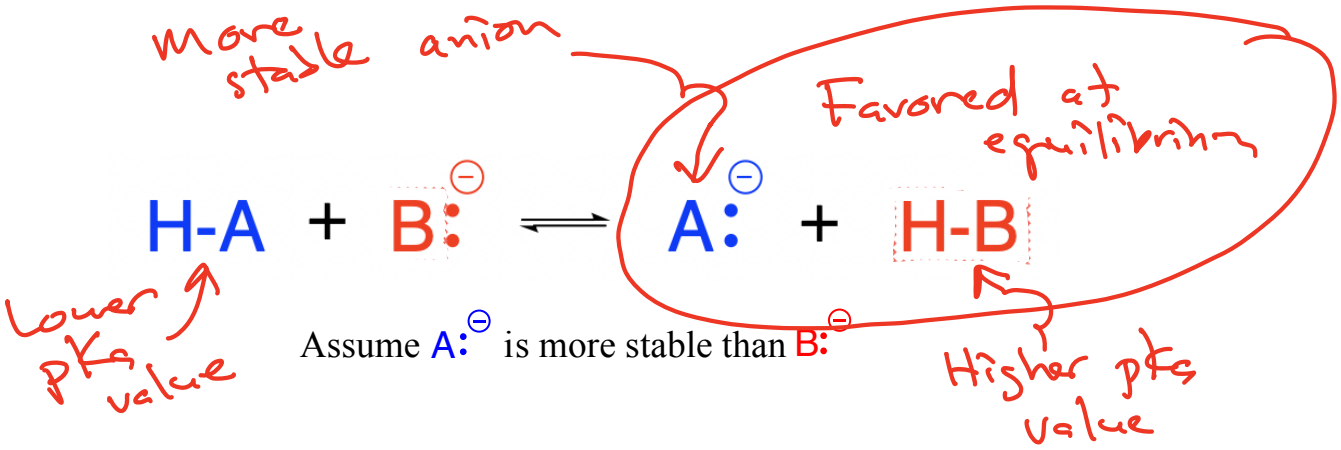


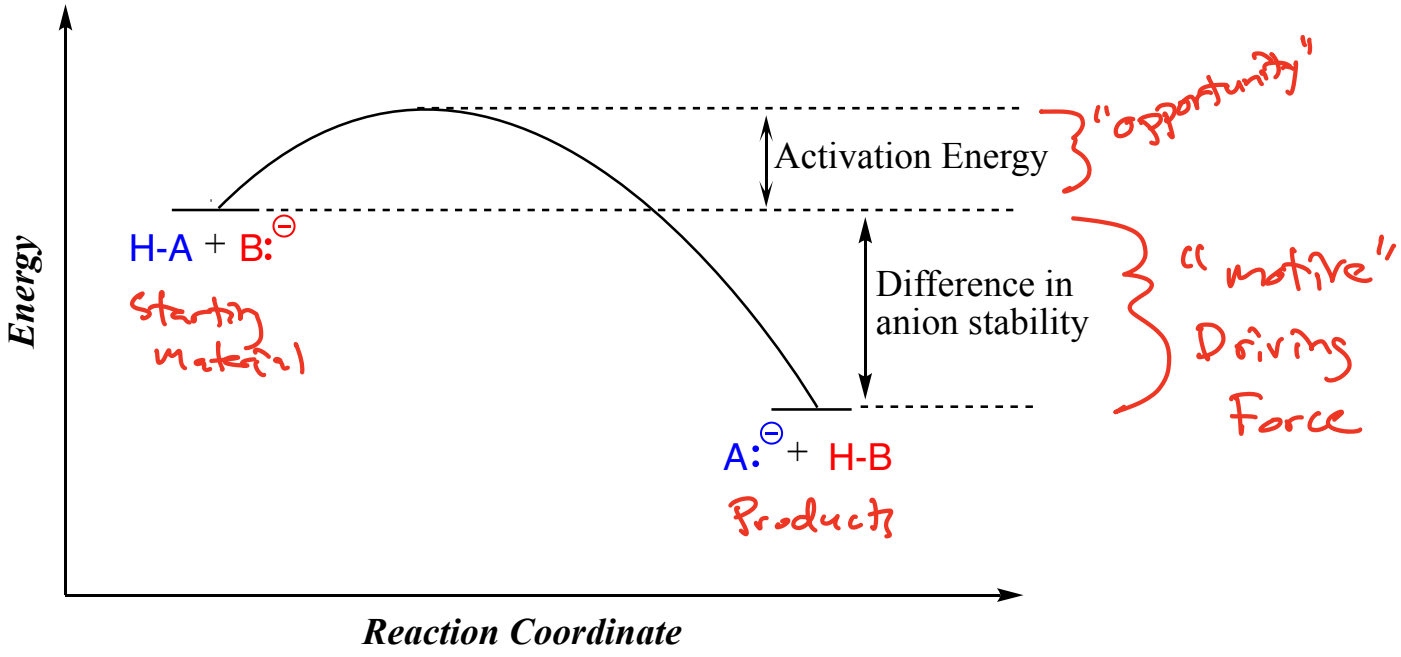
Resonance Delocalization Rule d)

Inductive Effect Rule e)

anion stability

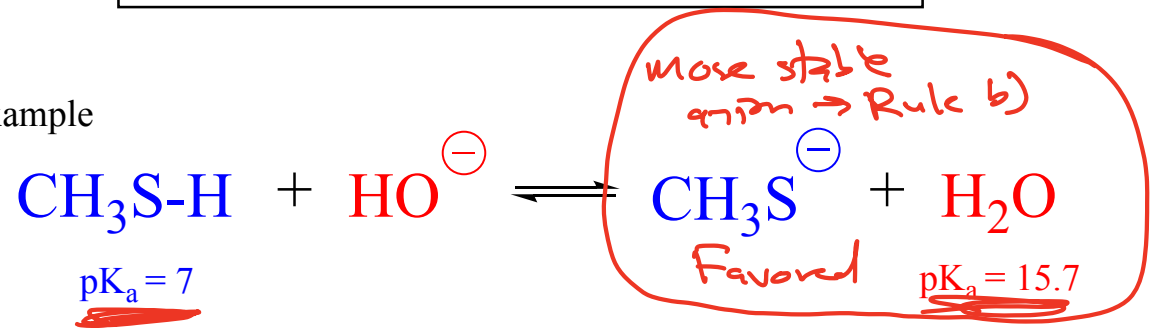
acid strength





$$K_{eq} = 10^{(pK_a\ \text{H-B} - pK_a\ \text{H-A})}$$

Example



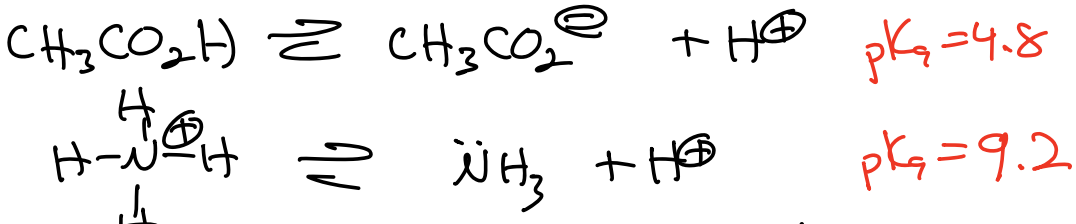
$$K_{eq} = 10^{(15.7 - 7.0)} = 10^{(8.7)}$$

New idea: How do pK_a and pH work together to determine predominant protonation states of acids?

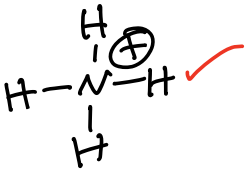
An acid is mostly protonated at a pH that is below its pK_a

An acid is mostly deprotonated at a pH that is above its pK_a

Examples:



Parent Acid → CH_3CO_2H ✓ ($pK_a = 4.8$)



✓ ($pK_a = 9.2$)

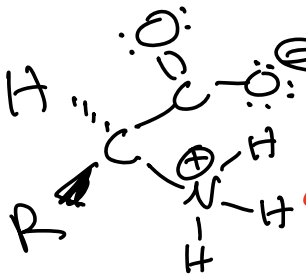
Forms Present at pH = 2.0: CH_3CO_2H ✓ $\oplus NH_4$

Forms Present at pH = 7.0: $CH_3CO_2^{\ominus}$ $\oplus NH_4$

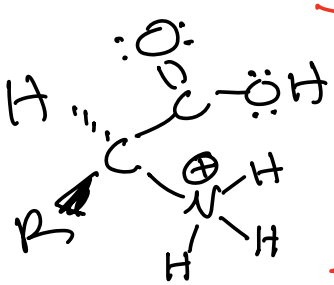
Forms Present at pH = 12.0: $CH_3CO_2^{\ominus}$ $:NH_3$ ✓

Application to important molecules → amino acids → same two groups we just saw

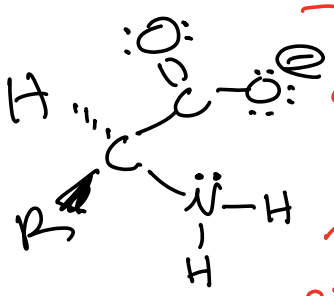
Form present at pH = 7.0



Form present at pH = 2.0



Form present at pH = 12.0



protonated

deprotonated

⇒ The $-CO_2H$ and $-\ddot{N}H_2$ forms are NEVER both present at any pH → Not possible!!

Why doesn't anyone get this right?

Amino acid

From Wikipedia, the free encyclopedia

This article is about the class of chemicals. For the structures and properties of the standard proteinogenic amino acids, see Proteinogenic amino acid.

Amino acids are organic compounds containing amine (-NH_2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.[1][2][3] The key elements of an amino acid are carbon (C), hydrogen (H), oxygen (O), and nitrogen (N), although other elements are