



How to estimate relative acid strengths



How do you
predict anion
stability?

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

2 important principles for predicting anion stability

- 1) Negative charge ($\ominus$) is neutralized by nuclear $\oplus$ charge.
- 2) Delocalizing negative charge ($\ominus$) over a larger area is better. → Golden Rule #5

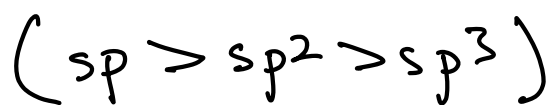
Rules for anion stability -

The anion is more stable when the negative charge ($\ominus$) 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



← 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)

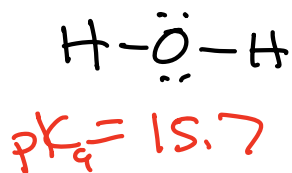
Operates
through sigma
bonds

{ nearby electronegative
atoms attract $\ominus$
charge and therefore
spread the $\ominus$ charge
onto more atoms

Examples

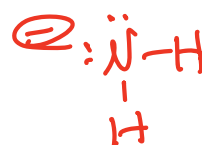
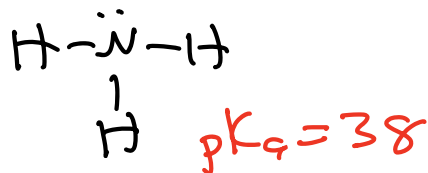
Rule a)

Ex.



more stable
anion

O is more electronegative



Rule b)



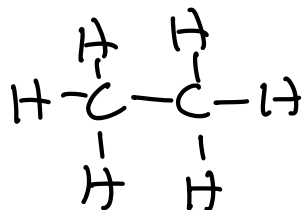
(Only compare atoms
in same column of
the Periodic Table)

$\text{p}K_a$	3.5	-7	-8	-9
	H-F	H-Cl	H-Br	H-I
	F^-	Cl^-	Br^-	I^-

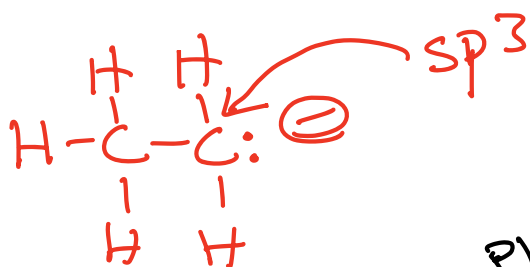
larger ion

acid strength

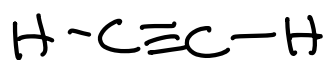
Rule c)



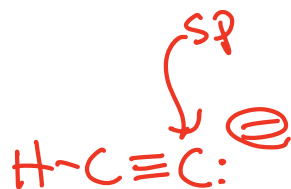
$$\text{p}K_a \cong 50$$



$$\text{sp}^3 \rightarrow 25\% \text{ s} \\ 75\% \text{ p}$$



$$\text{p}K_a = 25$$



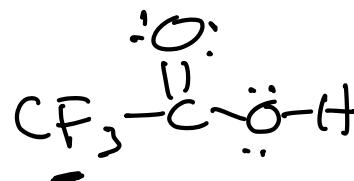
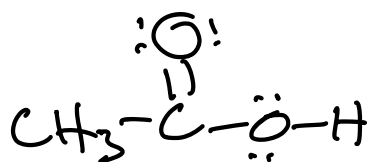
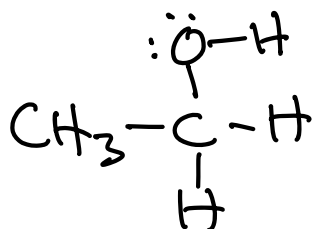
Places more
 $\ominus$ closer
to nucleus

More "s" $\rightarrow$

$$\text{sp} \rightarrow 50\% \text{ s} \\ 50\% \text{ p}$$

max stable anion

Rules d) and e)

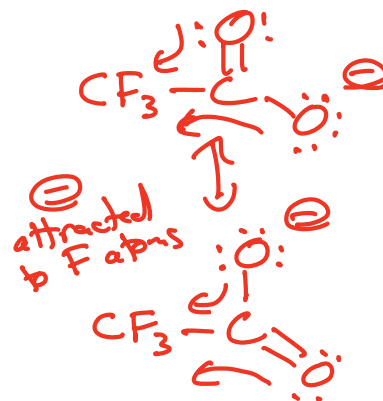
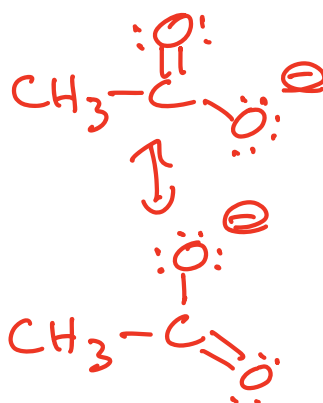
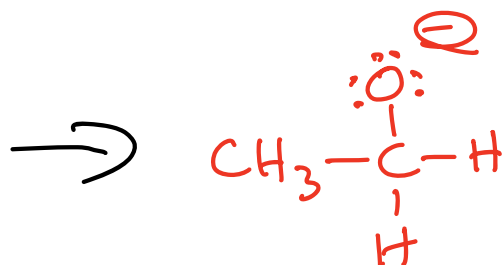


pK_a

15.9

4.8

0.1

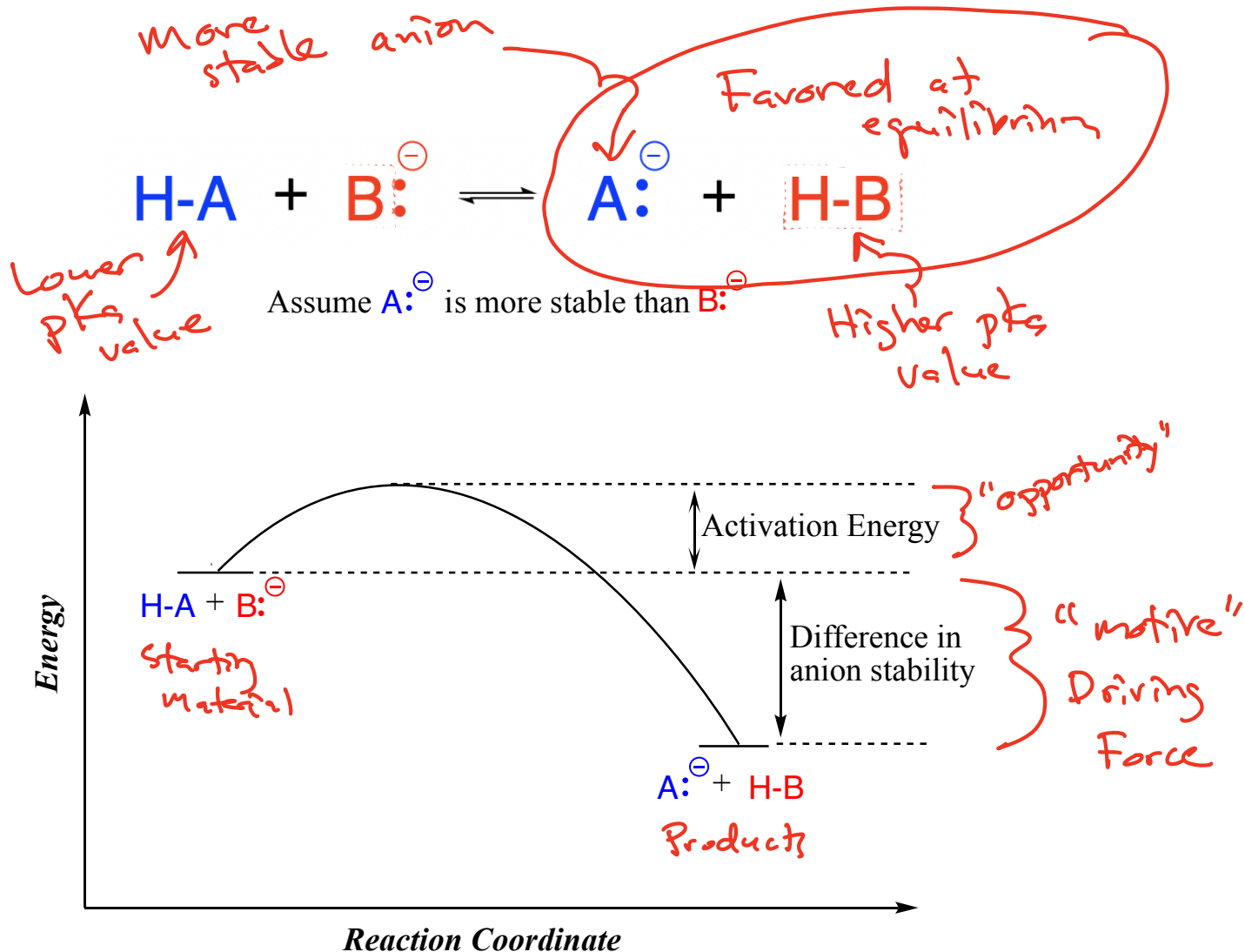


Resonance
Delocalization
Rule d)

Inductive
Effect
Rule e)

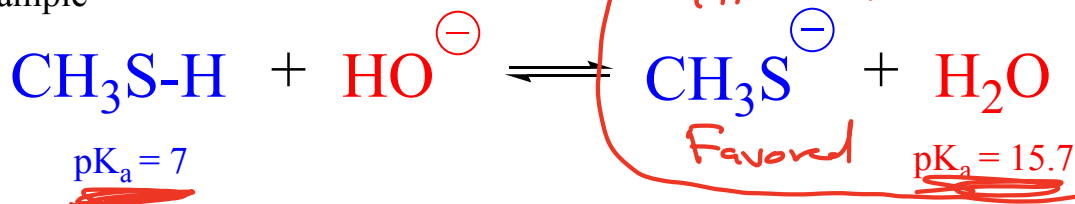
anion stability

acid strength



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

Example



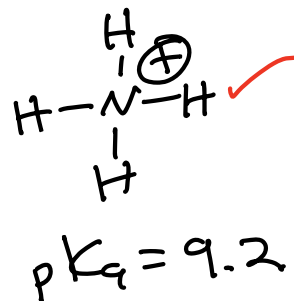
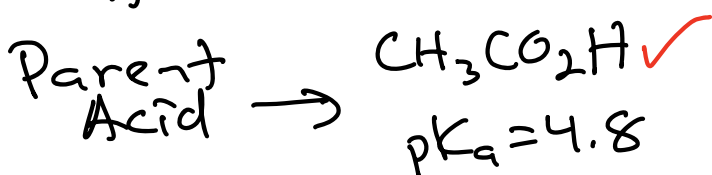
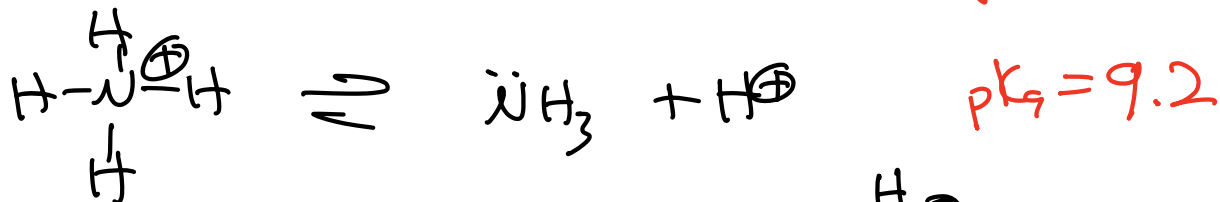
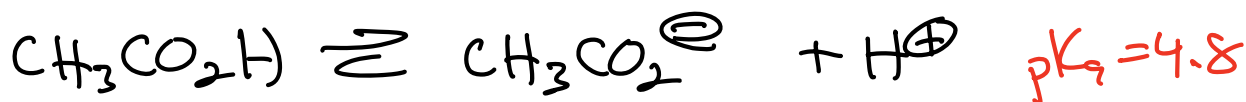
$$K_{\text{eq}} = 10^{(15.7 - 7.0)} = 10^{(8.7)}$$

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:



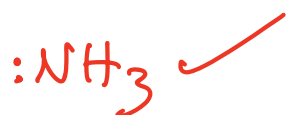
Forms Present
at $pH = 2.0$



Forms Present
at $pH = 7.0$

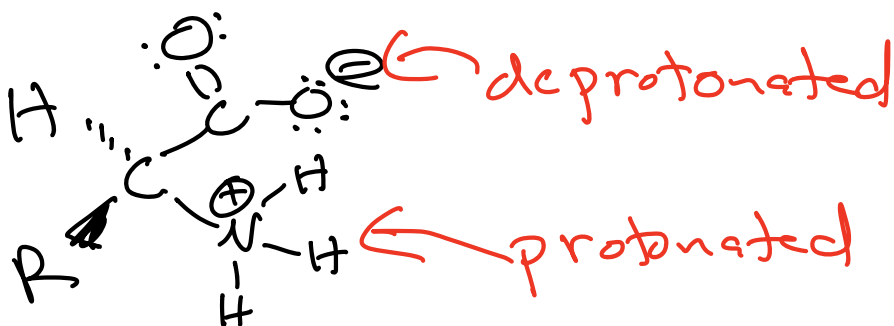


Forms Present
at $pH = 12.0$

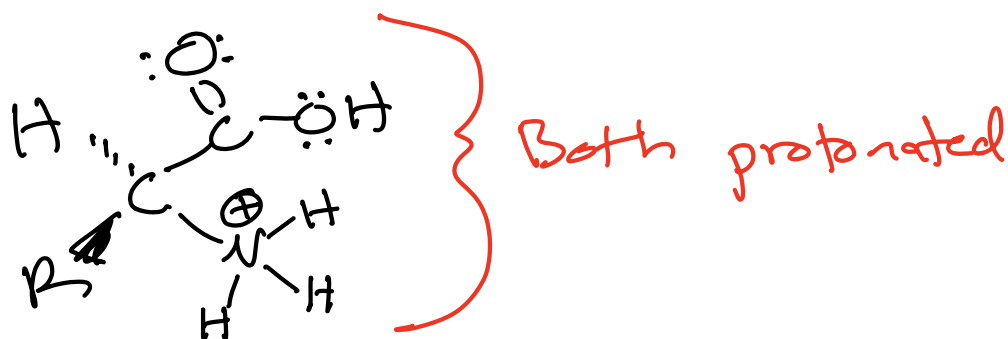


Application to important molecules $\rightarrow$ amino acids $\rightarrow$ same two groups we just saw

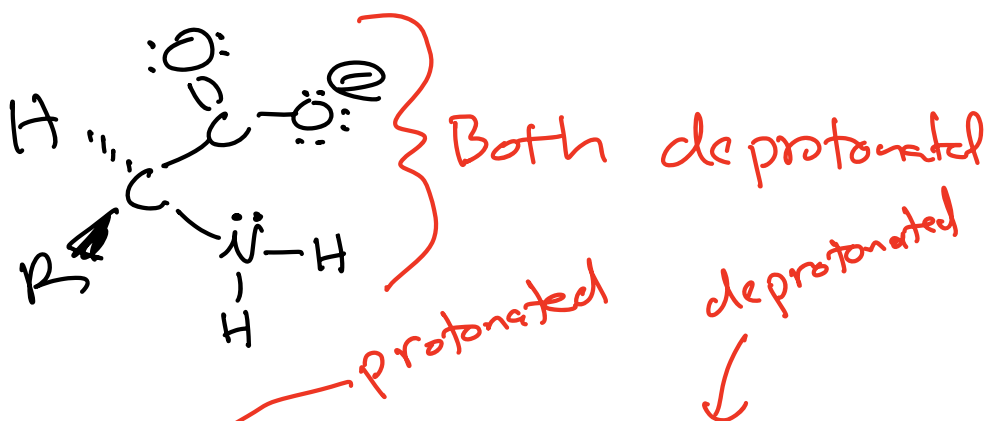
Form present at pH = 7.0



Form present at pH = 2.0



Form present at pH = 12.0



$\Rightarrow$ The $-CO_2H$ and $-NH_2$ forms are NEVER both present at any pH $\rightarrow$ Not possible!!

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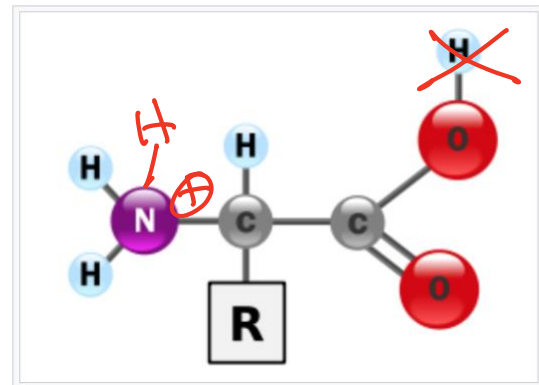
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Amino acid

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](#) (-NH₂) 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



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Amino acid structure

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Amino Acid Structure

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6.2.2 (a) Reactions of Amino Acids - ...

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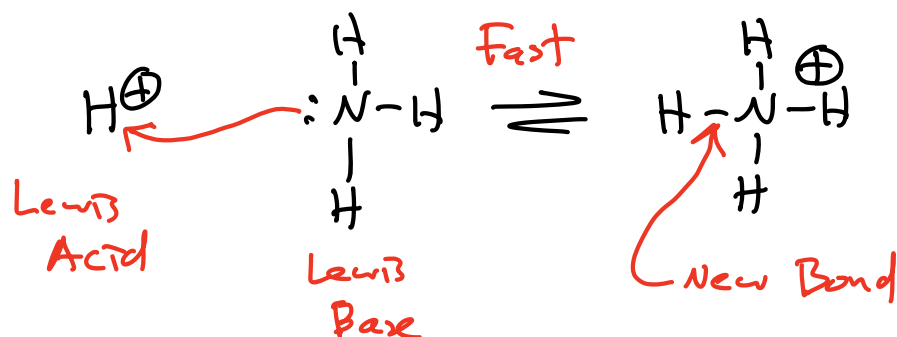
Image result for amino acid

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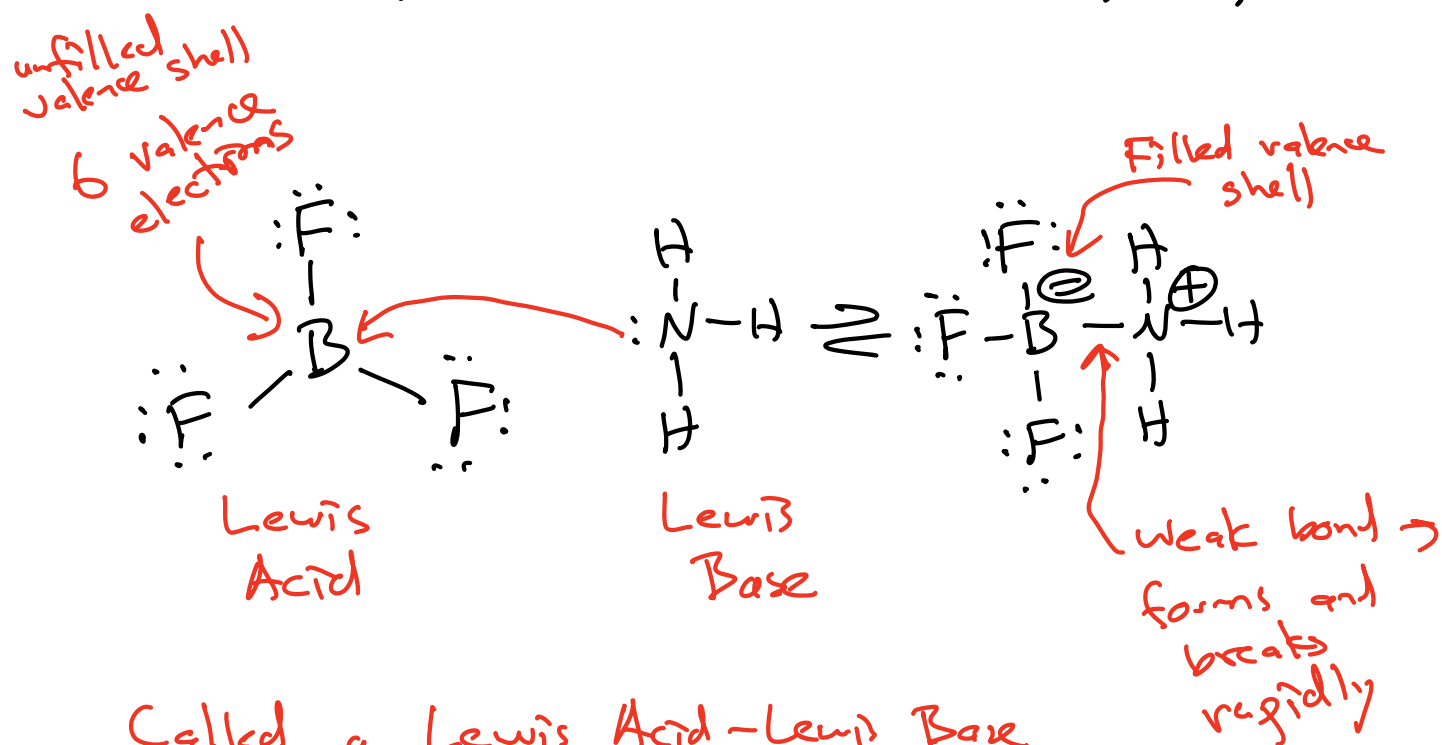
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Lewis Acid $\rightarrow$ accepts an electron pair

Lewis Base $\rightarrow$ donates an electron pair



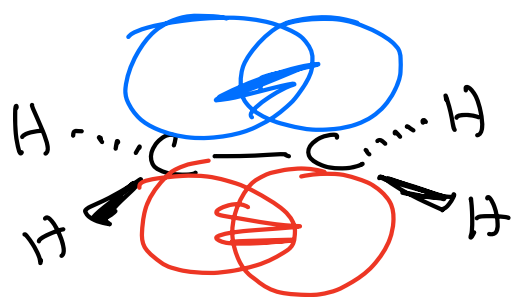
H^+ can be thought of as a Lewis acid, $\rightarrow$
but so can other species $\rightarrow$ atoms with an incomplete valence shell $\Rightarrow$ B, Al, Zn, Fe



Called a Lewis Acid-Lewis Base complex or "dative bond" or "coordinate covalent bond"



Electronic Structure of Alkenes



π bonds $\rightarrow$
overlap of
2p orbitals

Consequences of π bonds

1) π bonds cannot rotate

2) Electron density is above and below the bond axis so it is "available" to react with electron deficient atoms/molecules

Like a
Lewis
base

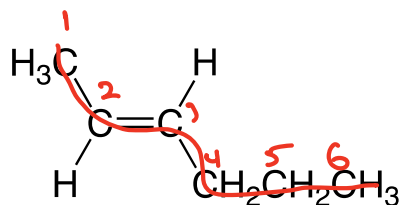
Naming Alkenes

General Directions:

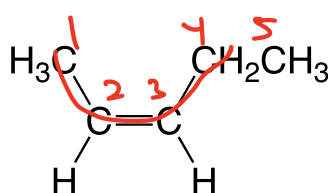
1. Locate longest continuous chain. ✓
2. Number the chain so the double bond gets the lowest possible number. ✓
3. For the parent chain name, use "-ene" not "-ane" as suffix and place a number to indicate the location of the double bond before the main chain name.
4. Make the suffix "-adiene", "-atriene", etc. if multiple double bonds are present.

cis/trans nomenclature – older chemical nomenclature, but still used commonly in biochemistry – most useful when each sp^2 atom of the double bond has an H atom.

1. Track the longest chain through the double bond ✓
 - a. **cis** if whole main chain is on the same side of the double bond. ✓
 - b. **trans** if chain emerges on opposite sides of the double bond. ✓



trans-2-hexene



cis-2-pentene

NOT

IUPAC

Naming Alkenes

General Directions:

1. Locate longest continuous chain. ✓
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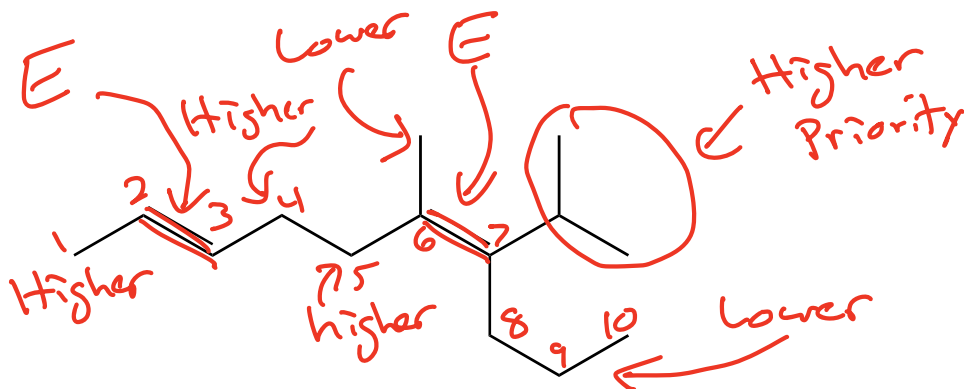
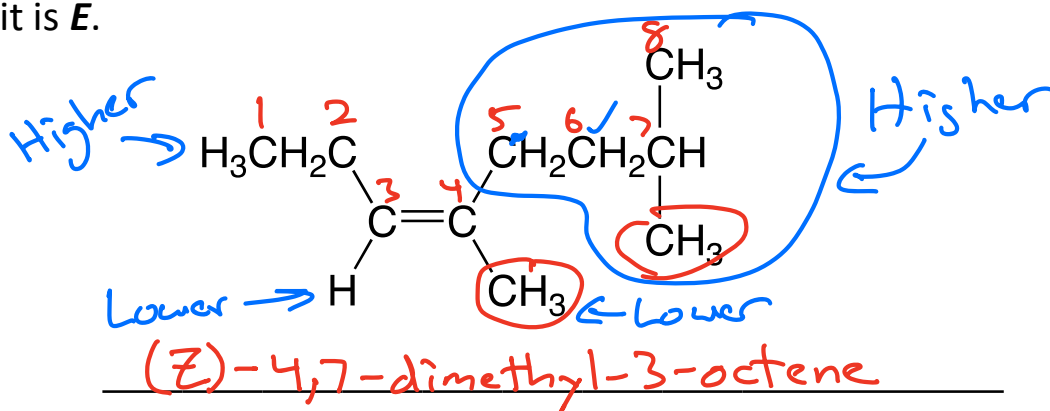
E,Z nomenclature - A general IUPAC nomenclature to names alkenes.



Z (zusammen) = same side, same side, same side

E (entgegen) = opposite side

5. On each carbon of the double bond rank the two groups according to the Cahn, Ingold, Prelog priority rules (*R* vs. *S* rules).
6. If both of the highest-ranking groups are on the same side of the double bond it is **Z**.
7. If both of the highest-ranking groups are on opposite sides of the double bond it is **E**.



(2E,6E)-7-isopropyl-6-methyl-2,6-decadiene

or **(2E,6E)-6-methyl-7-(1-methylethyl)-2,6-decadiene**