CHEM 30 UNIT A: THERMOCHEMISTRY

→ Open system: exchanges matter and energy w/ surroundings

→ Closed system: exchanges energy but not matter w/ surroundings

→ Isolated system: exchanges neither energy nor matter

→ During a chemical reaction, the bonds of the reactants must break, rearrange, and form new products

- → Breaking bonds = ~~exother~~ endothermic = absorbs energy (requires)
- → Forming bonds = exothermic = releases energy

~~→ Endothermic: energy released, breaking > forming~~

~~→ Exothermic: energy ab~~

→ Exothemic: energy released, breaking < forming   COLD   ex. photosynthesis ~~[illegible]~~

→ Endothermic: energy absorbed, forming > breaking   HOT   ex. combustion

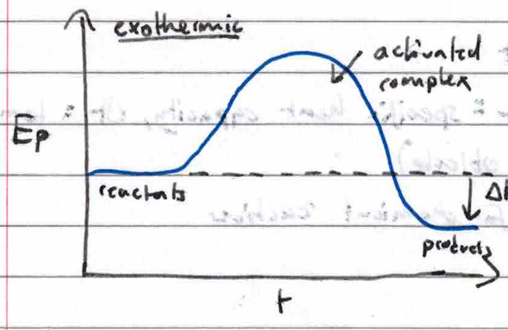
$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O + \boxed{2043.9 kJ}$ ← exothemic w/ products

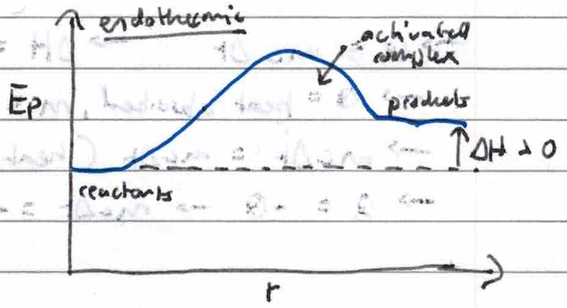
$N_2 + 2O_2$ ~~N_2O_4~~ $+ 11.1 kJ \rightarrow N_2O_4$ ← endothermic w/ reactants

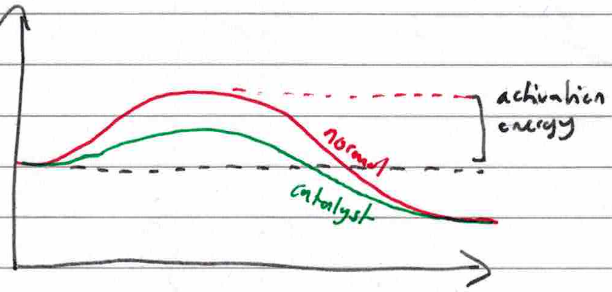
$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \quad \Delta H = -2043.9 kJ$ ← exothemic $\Delta H < 0$

$N_2 + 2O_2 \rightarrow N_2O_4 \quad \Delta H = +11.1 kJ$ ← endothermic $\Delta H > 0$

→ collision theory: chemical species collide and transfer energy during a chemical reaction







→ activation energy is needed for the reaction to take place

→ A catalyst reduces the amount of activation energy required, but doesn't speed up the reaction

→ Collision theory steps
I. Particles move around and collide
II. If the energy and orientation are correct, a transition state is formed
III. Atoms in the transition state rearranged, bonds are broken
IV. The new particles move away from each other

→ Activation energy is a barrier that must be surpassed for the equation to take place

→ Catalysts provide an "alternate pathway" to lower the activation energy
→ Catalysts are <u>not</u> used in the reaction

reverse
→ Photosynthesis : $6CO_2 + 6H_2O + \text{energy} \rightarrow C_6H_{12}O_6 + 6O_2$ ($\Delta H > 0$) endo
→ Cellular respiration : $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O + \text{energy}$ ($\Delta H < 0$) exo

→ Hess's law : regardless of the "route" taken, ΔH remains the same for the total reaction
→ $\Delta_r H = \Delta_1 H + \Delta_2 H \ldots$ or $\Delta_r H = \Sigma \Delta_r H$

→ $\Delta H°$ can be predicted using a table
→ $\Delta H = \Sigma_{\text{products}} (n \Delta_f H_m) - \Sigma_{\text{reactants}} (n \Delta_f H_m)$
→ Total energy = energy (products) − energy (reactants)

→ Spesfic heat capacity : how "difficult it is to heat something"
→ Water = 4.19 J/g•c

→ $Q = mc\Delta t$ → $\Delta H = mc\Delta t$
→ Q = heat absorbed, m = mass, c = specific heat capacity, Δt = temperature change
→ $mc\Delta t = mc\Delta t$ (heat between objects)
→ $Q = -Q$ → $mc\Delta t = -mc\Delta t$ for chemical reactions

- The pH scale measures how acidic or basic something is
  - ↳ logarithmic scale from 0 (acidic) - 14 (basic)
  - ↳ 7 is neutral (ex. H_2O)
  - ↳ PH measures the hydrogen ions (H^+) in the substance:

$pH = -\log_{10}[H^+]$ / $PH = -\log_{10}[H_3O^+]$ $10^{-pH} = [H_3O^+]$

$pOH = -\log_{10}[OH^-]$ $10^{-pOH} = [OH^-]$

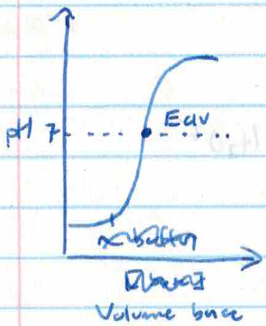
$pH + pOH = 14$

  - ↳ Strong acids and bases dissociate completely (ionize completely)
    - ↳ therefore $[acid] = [H_3O^+]$ and $[base] = [OH^-]$
  - ↳ The number of decimal places in a pH value is the number of significant digits in the concentration of $[H_3O]^+$
    - ↳ Same for pOH

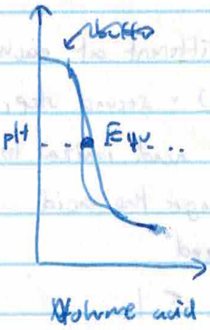
- When a strong acid or base ionizes, the reaction is not equilibrium
  - ↳ Acide : $HA + H_2O \rightarrow H_3O^+ + A^-$
  - ↳ Base : BOH ~~$+ H_2O$~~ $\rightarrow B^+ + OH^-$
- When a weak acid partially ionizes, an equilibrium is formed
  - ↳ Acid : $HA + H_2O \rightleftharpoons H_3O^+ + A^-$
  - ↳ $K_a = [H_3O^+][A^-] / [HA]$
  - ↳ Base : ~~$BOH \rightleftharpoons BH + OH^-$~~ $B^- + H_2O \rightleftharpoons BH + OH^-$
  - ↳ $K_b = [BH][OH^-] / [B^-]$
- These constants can be used to calculate concentrations, like K_a

- A buffer is a relatively equal mix of a weak acid and base [conjugate pair]
  - ↳ If a strong acid or base reacts with the buffer, it will react with the weak base/acid and not the water
  - ↳ The pH won't change much in the buffer region
  - ↳ Buffers can be both basic and acidic
  - ↳ Buffers are equilibrium systems, and follow Le Chatelier's principle
  - ↳ The equilibrium reaction for a buffer is the same as it's ionization reaction
  - ↳ Changes in pH $[H_3O^+]$ will cause the system to "correct itself"

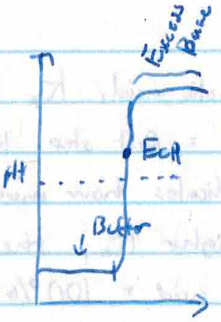
Titrations



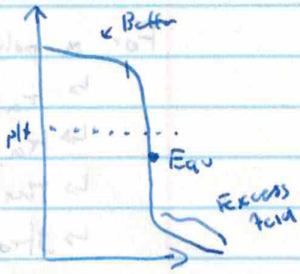
Strong acid with strong base



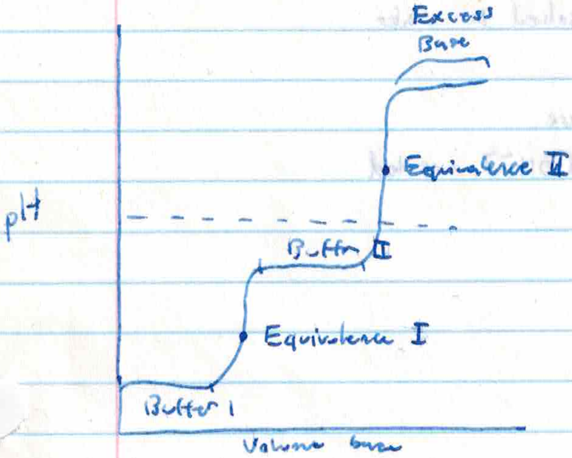
Strong base with strong acid



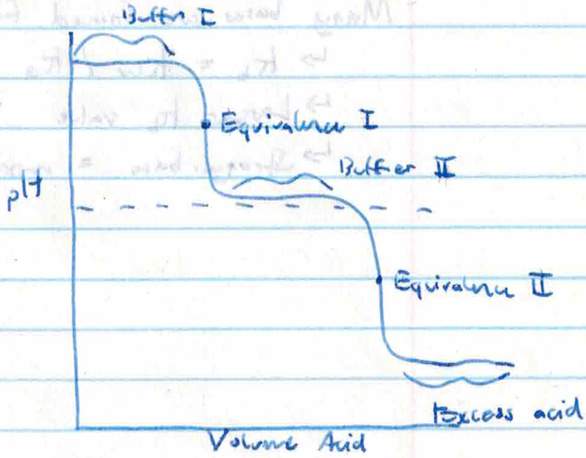
Weak acid with strong base



Weak Base with strong acid



Titration of Acid w/ Base



Titration of Base w/ acid

↳ Number of bumps = Number of H^+ available

- Water can sometimes ionize itself: $2H_2O \rightleftharpoons H_3O^+ + OH^-$
    - ↳ This forms an equilibrium state
    - ↳ $K_w = [H_3O^+][OH^-]$ ionizing constant of water (1×10^{-14} at 25°C)
    - ↳ The forwards reaction is <u>endothermic</u> $\Delta H > 0$

- Weak acids and bases use simplified equation for K_a and K_b
    - ↳ Acid: $HA \rightleftharpoons H^+ + A^-$ (simplified, weak acids)
    - ↳ $K_a = [H^+][A^-]/[HA]$
    - Base:

For a polyprotic acid, K_a is different at each step
- ↳ $K_a(1)$ = first step, $K_a(2)$ = second step, etc
- ↳ K_a indicates how much an acid ionizes to form H_3O^+
- ↳ The higher K_a, the stronger the acid
- ↳ Strong acid = 100% ionized
- ↳ Weak acids have a $K_a < 1$
- ↳ Higher K_a, better conductivity

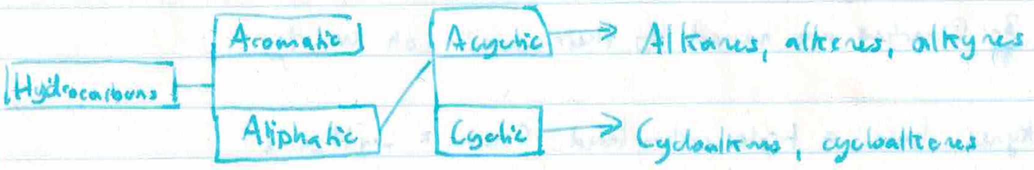
- Many bases are formed from salts dissolved in water
  - ↳ $K_b = K_w / K_a$
  - ↳ Larger K_b value = stronger base
  - ↳ Stronger base = more ionization, $[OH^-]$ created

Organic Chemistry

- Carbon forms many organic compouns (90% of all)
  - ↳ Carbon has 4 valence electrons = 4 strong covalent bonds
  - ↳ Can create stable bonds with itself
  - ↳ Strong bonds often stay together in chemical reactions

- Saturated hydrocarbons are formed only of single bonds
  - ↳ when C forms 4 single bonds, it becomes a straight - chain alkane
  - ↳ Single bonds permit rotation
- Unsaturated hydrocarbons have double and triple bonds
  - ↳ Double bonds change the geometry of the molecule
  - ↳ They make the molecule more rigid

- Organic compounds contain carbon, hydrogen, and a few other elements (oxygen)
  - ↳ Simplest organic compounds are hydrocarbons : hydrogen and carbon
    - ↳ Can be grouped into families : alkanes, alkenes, alkynes, cycloalkanes
  - ↳ Organic compounds often have a carbon "backbone"
  - ↳ Straight - chain and cyclic hydrocarbons : aliphatic compounds
  - ↳ More complex compounds = aromatic compounds



- ↳ Alkans : single carbon bond
- ↳ Alkense : double carbon bond
- ↳ Alkynes : triple carbon bond
- ↳ Structural isomer : different molecules with the same formula

- ↳ Cyclo : carbons form a ring
- ↳ Hydrocarbon names end in ane, ene, and yne.

- Organic compounds include glucose, proteins, and fats
  - ↳ Nitrogen as minor element = amino acids (building blocks for proteins)

- Alkans only have single carbon bons (form = C_nH_{2n+2})
  - ↳ Prefix = number of carbon atoms in longest chain ....→ meth = 1, eth = 2, prop = 3, but = 4
- Alkanes with side chains (stuff sticking out)
  1. Name normally (longest carbon chain)
  2. Each hydrocarbon sidechain = amount of C + -yl prefix
  3. List sidechain names alphabetically
  4. Number the position of the sidechain (start at closest end) (use commas if repetition)
  5. Use prefixes di, tri to indicate multiple identical sidechains

- Alkenes have at least one carbon-carbon double bond (form = C_nH_{2n})
  1. Find the parent chain, name with -ene suffix
  2. Number the (smallest) position of the double bond (ex. hept 2-ene)
     - ↳ If more than one, use greek prefixes . position
  3. Number sidechains as per normal (ex. 2nd- methyl hept-2-ene)

- Cyclic alkenes form a ring structure (Form = C_nH_{2n-2})
  1. Parent chain = ring structure. These structures have -cyclo prefix
  2. If the endpoints of the double bonds have bonds, one of the endpoints becomes 1- carbon
     - ↳ Else, just number in order
  3. Branches are named by their position on the ring

- Alkynes have a triple carbon bond (form = C_nH_{2n-2})
  - ↳ Alkynes have the same naming conventions as alkenes, but have the suffix -yne

- Cyclic alkanes have a circular structure and single bonds (form = C_nH_{2n})
  - ↳ cyclic alkanes use the prefix -cyclo, but are named the same as alkanes
    - ↳ ex. 1,1 - dimethyl cyclohexane

Benzene

↳ Benzene doesn't have true double and single bonds

↳ Oscillates between the two positions

↳ Cyclic alkene, formula C_6H_6

↳ When a benzene ring has one sidechain bond with another compound, it is called a phenyl group (Toluene = benzene + methyl gr

- Aromatics are complex molecules with cyclical structures (like benzene)
  - ↳ Furan: C_4H_4O (also in an oscillatory state)
- Aromatic compounds are named with the benzene ring as the parent chain
  - ↳ groups are numbered like normal
  - ↳ benzene ring as group w/ one group = -phenyl prefix

- Skeletal isomer: differs how the carbon atoms are attached to one another
- Position isomer: position of group on parent chain (ex. butan-1-ol and butan-2-ol)
- Functional group isomer: different functional groups
  - ↳ ex. propan-1-ol vs. methoxyethane

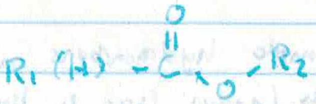
- Functional group: group that defines the properties of the molecule
  - ↳ active sites for chemical reaction
  - ↳ each group is unique: compounds can be classified
  - ↳ serve as base for naming compounds

Alchohols: $R-OH$

Amines: $R-NH_2$

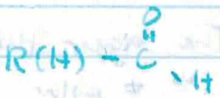
Ethers: R_1-O-R_2

Esters:



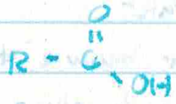
$R_1(H)-C(=O)-O-R_2$

Aldehydes:



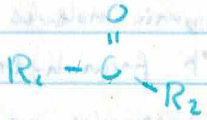
$R(H)-C(=O)-H$

Carboxylic acids:



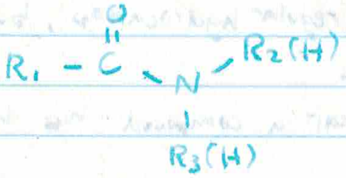
$R-C(=O)-OH$

Ketones:



$R_1-C(=O)-R_2$

Amides:



$R_1-C(=O)-N(R_2(H))(R_3(H))$

→ R_1, R_2, R_3 can't be the same group

→ R(H) means that replacing the group with H won't seriously alter the structure

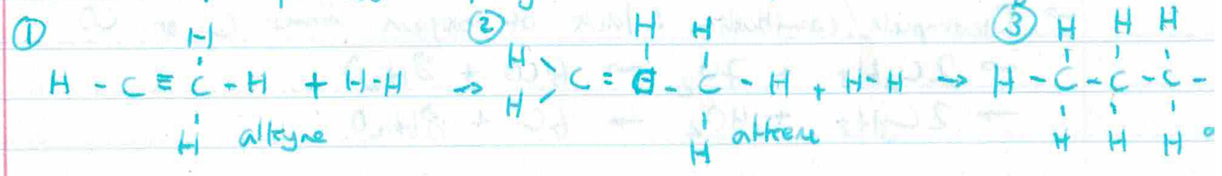
Alkanes can undergo substitution reactions with F_2, Cl_2 Br_2 I_2
↳ Except for F_2, this process requires energy
↳ To name the product, add the halogen prefix and use numbering
↳ ex. 1,2 dibromo ethane
Alcohols have an $-OH$ functional group attached to the parent chain
↳ Primary: attached to a C at the edge of the chain
↳ Secondary: attached to a C on the middle (no other group at position)
↳ Tertiary: attached to a C that has another group attached to it
- Alcohols are alkanes, and follow the alkane naming rules
↳ Replace the "e" with "ol" to name the alcohol
↳ ex. 2-methylpropan-1-ol (1 and 2 indicate positions)

- Carboxylic acids contain a $-COOH$ ($\overset{\overset{O}{\|}}{C}-OH$) group
↳ to name, replace the "e" in alkane with -oic acid

- Esters are formed by the reaction of a carboxylic acid and an alcohol
↳ have the functional group $-COO-$
↳ to name: first name the alkyl group attached to the O (the one that replaces H
↳ then name the hydrocarbon attached to the C in the ester group
with the suffix -oate
↳ ex. propyl ethanoate, methyl butanoate

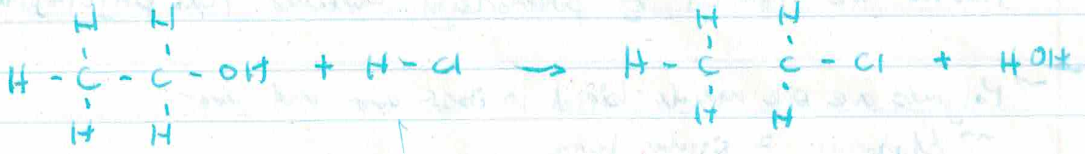
- Simple hydrocarbons are usually non-polar
↳ London force is the primary force that determines boiling point
↳ The bigger the molecule, the higher the forces and melting point
↳ ≠ polar = ≠ soluble in water
- Some organic molecules are slightly polar because of $-O-$ and $-C=O$ groups
↳ Can't form hydrogen bonds with each other
↳ polar molecules are stronger than regular hydrocarbons, but weaker than compounds with hydrogen forces
↳ Having an $-OH$ group means that a compound has hydrogen forces
↳ Higher boiling point
↳ Carboxylic acids have all three forces = high boiling point
↳ Aromatics also usually have a high boiling point
↳ Benzene on its own isn't soluble in water; the groups define the solubility

- Addition reaction: atoms are added to unsaturated bond in hydrocarbon
  - ↳ Involve alkenes and alkynes (not alkanes)
- Hydrogenation: Hydrogens are added to unsaturated bonds
  - ↳ Two steps (possibly) Alkyne → Alkene, alkene → alkyne

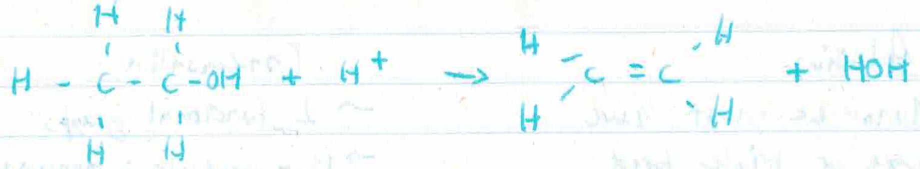


↳ Halogenation: Halogens (Cl_2, ~~to~~Br_2) get added to unsaturated bonds
↳ Hydrohalogenation: Hydrogen halide (HCl, HBr) gets added to unsaturated carbon bond

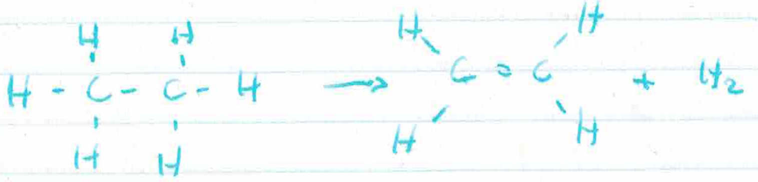
→ Substitution reaction: one atom or group is replaced with another atom or group
↳ May have multiple products (different replacement positions)



- Elimination: molecule looses groups or atoms
  - ↳ dehydration: water is removed from an atom



↳ dehydrohalogenation: hydrogen and halogen atoms are removed from mo
↳ Dehydrogenation: Hydrogen atoms are removed



→ Combustion: exothermic reaction that produces oxides and heat
  → $2H_2 + O_2 \rightarrow 2H_2O$
  → $2S + 3O_2 \rightarrow 2SO_3$
  → $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$
→ Incomplete combustion: lack of oxygen forms C or CO
  → $2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O$
  → $2C_3H_8 + 4O_2 \rightarrow 6C + 8H_2O$

→ Solvent extraction: separating chemicals using solvents
1. Solvents have different solutes (ex. A → water, B → oil)
2. Solvents can't mix, so they form layers
3. The layers should be easy to separate

→ Use a spout to drain layer by layer

→ Fossil fuels are exothermic: they produce heat and energy
→ Plastics are formed by polymerizing molecules (ex. polyethylene)

→ Polymers are one molecule joined to itself over and over
  → Monomer = singular form
  → Natural and synthetic polymers
  → Homopolymers = one monomer, copolymers: 2 monomers

Addition	Condensation
→ Monomers must have double or triple bond	→ 2 functional groups
→ No by-products	→ By-products: ammonia, water, HCl
→ Addition of monomers makes polymers	→ Condensation → monomers