Final Exam Review – Chem 1040

Wavelength and Energy

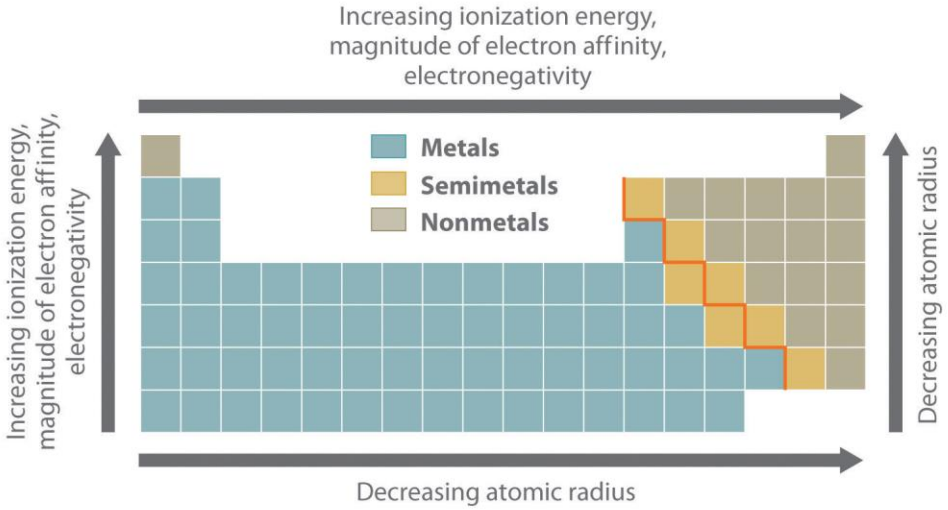
- Wavelength and frequency are related through the following equation: **$c = \lambda * v$**
    - C = speed of light at 3.00*10^8
    - λ = wavelength in nm
    - v= frequency in Hz
- To find the energy we use the following equation: **$E = h * v$**
    - E = energy in joules
    - h= Plank's constant (6.63*10^-34)
    - V= frequency in Hz

Quantum Numbers

- Principle quantum number (n): represents the main energy level of an atom's electron by a number (1,2,3...) or letter (k, l, m, n...), increasing values of n indicates an increasing value of energy
- Angular momentum (l): tells us the shape of the orbital each associated with a different shape. **l=(n-1)**
    - l= 0= spherical= s
    - l= 1= dumb-bell= p
    - l= 2= clover-live= d
    - l= 3= clover & dumb-bell= f
- Magnetic quantum number (ml): determines the number of permitted orbitals in any group – ranges from –l to +l
- Spin quantum number (ms): limits the number of electrons per orbital, only 2 values are possible - -½ and +½
- Pauli exclusion rule: no 2 electrons can have the same set of all four quantum numbers
- Hund's rule: electrons must be distributed in orbitals to yield maximum numbers of unpaired electrons
- REMEMBER COPPER (Cu) AND CHROMIUM (Cr) – 1 AWAY FROM FULL OR HALF D ORBITAL, ARE DIFFERENT AS THEY HAVE FULL 4S ORBITALS!

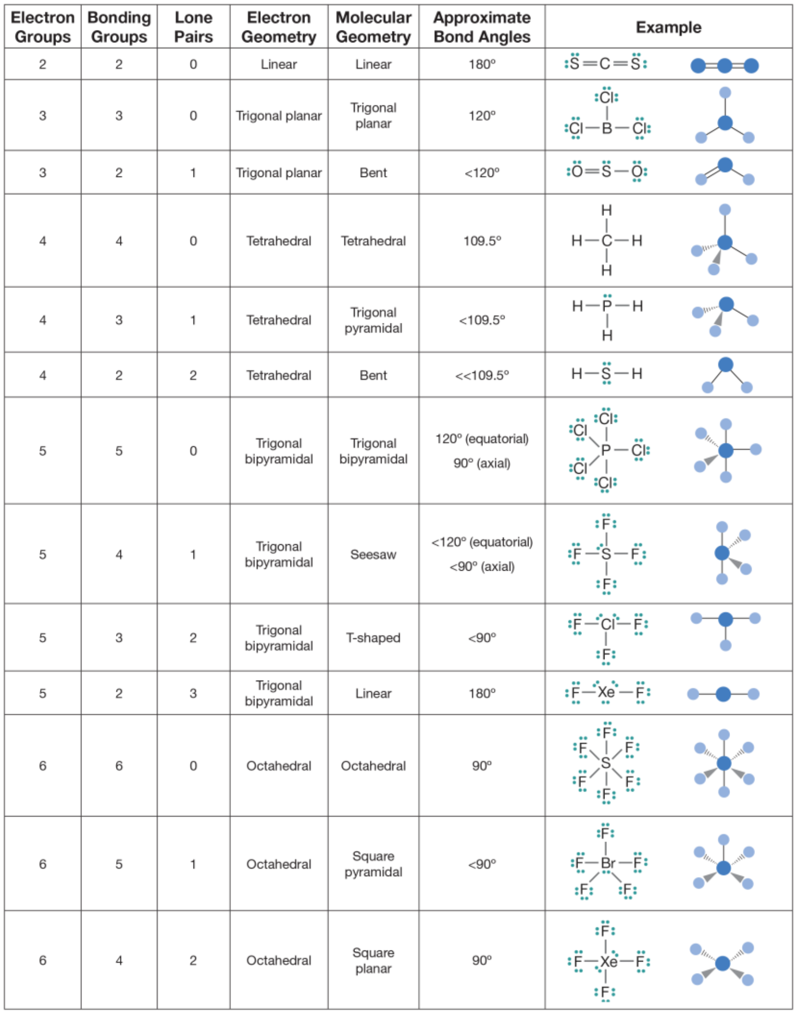
Atomic trends

- Isoelectric: atoms with the same electron configuration but different ions (Na+ and Ne)
- Diamagnetism: not attracted to or slightly repelled by magnetic field (all electrons are paired)
- Para-magnetic: attracted by magnetic fields from unpaired electrons, the more unpaired the electron – the higher the magnetism value



- Size and charge of ions: +vely charged ions are smaller, -vely charged ions have a larger radius (nuclear charge, # of electrons, valence orbital)

Molecular Geometry and Hybridization



Electron Groups	Bonding Groups	Lone Pairs	Electron Geometry	Molecular Geometry	Approximate Bond Angles	Example
2	2	0	Linear	Linear	180°	
3	3	0	Trigonal planar	Trigonal planar	120°	
3	2	1	Trigonal planar	Bent	<120°	
4	4	0	Tetrahedral	Tetrahedral	109.5°	
4	3	1	Tetrahedral	Trigonal pyramidal	<109.5°	
4	2	2	Tetrahedral	Bent	<<109.5°	
5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	120° (equatorial) 90° (axial)	
5	4	1	Trigonal bipyramidal	Seesaw	<120° (equatorial) <90° (axial)	
5	3	2	Trigonal bipyramidal	T-shaped	<90°	
5	2	3	Trigonal bipyramidal	Linear	180°	
6	6	0	Octahedral	Octahedral	90°	
6	5	1	Octahedral	Square pyramidal	<90°	
6	4	2	Octahedral	Square planar	90°	

- Molecular geometry: general shape of a molecule as determined by the relative positions of the atomic nuclei
- VESPER Theory: predicts the shape of molecules based on the assumption that valence shells are positioned so that electrons will be as far away as possible from each other
- Formal charges: the charge on each individual atom based on their charge on the period table and how many electrons they own in the compound
- Hybridization and geometry
    - AB2 – linear -- sp
    - AB3 – trigonal planar – sp2
    - AB4 – tetrahedral – sp3
    - AB5 – trigonal bipyramidal – sp4
    - AB6 – octahedral – sp5
    - Essentially to find the hybridization just find the number of electron domains and subtract '1'
- Sigma bonds: single bonds
- Pi bonds: double and triple bonds

Stoichiometry

(*always try to use moles*)

- For solids: **#moles = mass(g) / molar mass**
- For liquids: **concentration = number of moles / volume (L)**
    - therefore, **n = concentration*volume**
- For gases: PV=nRT
- To find the number of moles for a multi-step reaction:
    - Find a product in the 1st equation that is a reactant in the 2nd equation
    - Solve for the number of moles of the product in the 1st equation
    - Use that same number of moles to find the number of moles of the desired product
- To find the limiting reagent:
    - Convert the masses you are given into moles using molar mass
    - Take note of the reaction coefficient
    - Divide the number of moles calculated by the reaction coefficient
    - The number that is smaller is the limiting reagent
- To find % yield: **%yield = (actual/theoretical)*100**
    - Use the actual yield given in the question
    - Calculate the theoretical yield using the limiting reagent
    - Plug the numbers into the formula

Chemical Reactions

- Electrolyte solutions
    - Strong electrolyte: the solution exists entirely as ions, which can be salts, strong acids and strong bases

  - Weak electrolytes: solution is partially ionized which can be weak acids or weak bases
  - Non-electrolytes: solutions that do not contain ions – mostly organic compounds
- The equations
  - Molecular equations: the equation in which the products and reactants are written as compounds rather than ions
  - Complete ionic equations: chemical equations in which the compounds are written as individual ions in the solution
  - Net ionic equations: the complete ionic equation with spectator ions cancelled
- Precipitate reactions
  - A precipitate will form when there is a compound in the products that is insoluble

Acids and Bases

- Arrhenius acid: supplies H+
- Arrhenius base: supplies OH-
- Bronsted-Lowry acid: gives a H+ (proton donor)
- Bronsted-Lowry base: receives a H+ (proton acceptor)
- Strong acids: acids that fully dissociate in water (6 to remember: HCL, HI, HBr, HNO3, HCLO4, H2SO4)
- Strong bases: bases made with OH and an alkali metal or alkali earth metal (group 1 or 2) -- 8 to remember: LiOH, NaOH, KOH, RbOH, CsOH, Ca(OH)2, Ba(OH)2, Sr(OH)2
- Weak acid/base: every other acid/base that isn't strong
- Lewis acid: accepts a pair of electrons for the Lewis base
- Lewis base: gives a pair of electrons to the Lewis acid

pH= -log[H30+] . **pOH = -log[OH-] .** **14 = pOH + pH**

*when you have 2 sig figs in the concentration, you need to have 2 decimal places in the pH

pKa = -logKa **K = 10^-pka**

- Amphoteric: it can act as either an acid or a base depending on the situation (ex. Water)
  - b/c water is amphoteric it can self-dissociate or self-ionize, and pure water contains equal amounts of H30+ and OH-

Kw = 1.00 *10^-14 = (ka)(kb)

- When finding the stoichiometric concentration of acids and bases:
  - In a strong acid the nominal concentration is the same as the concentration of H3O+
  - Strong bases are different b/c sometimes you have 2 moles of OH- (ex. Ca (OH)2)
    - In this case, you will multiply the nominal concentration by the coefficient (for Ca (OH)2 you would multiply it by 2)

  - Weak acids do not fully dissociate in water, so their concentration in calculated by using: **Ka = x^2 / (nominal concentration-x)**, where x = [H3O+]
  - Weak bases do not fully dissociate in water, so their concentration is calculated in a similar way: **Kb = y^2 / (nominal concentration–y)**, where y = [OH-]

*in both calculations for concentrations of weak acids and weak bases you can use approximation instead of using the quadratic formula!

Nominal concentration / ka or kb >> 100

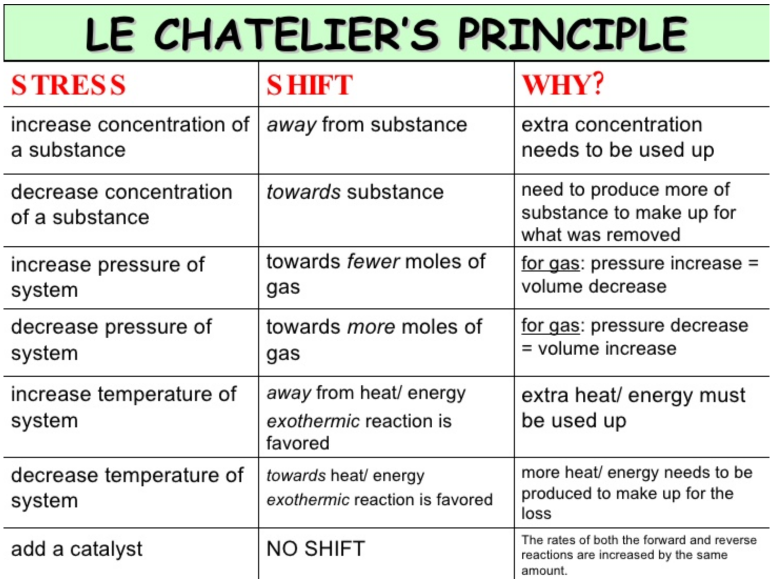
- In weak acids:
  - A larger Ka means a stronger weak acid
  - A smaller Ka means a weaker weak acid
- In weak bases:
  - A larger Kb means a stronger weak base
  - A smaller Kb means a weaker weak base
- In order to determine the Keq of a reverse reaction:
  - Flip the reaction and see if you can find a Ka or Kb value for the reaction
  - If you can, the new keq is equal to 1/Ka or Kb that you found

Equilibrium

Kc = ([products]^reaction coefficient) / ([reactants]^reaction coefficient)

remember that pure solids are not included in this equation

- When Kc is very larger the reaction goes to completion and the products are favored
- When Kc is very small the reaction favors the reactants
- If we reverse a reaction, the k value gets inverted and becomes 1/K
  - Q is calculated using the Kc equation at any other point in the reaction when it is not at equilibrium
  - Q = K, at equilibrium
  - Q < K, reaction is moving from left to right until Q = Kc (not enough product)
  - Q > K, reaction is moving from right to left until Q = Kc (too much product)



LE CHATELIER'S PRINCIPLE

STRESS	SHIFT	WHY?
increase concentration of a substance	*away* from substance	extra concentration needs to be used up
decrease concentration of a substance	*towards* substance	need to produce more of substance to make up for what was removed
increase pressure of system	towards *fewer* moles of gas	for gas: pressure increase = volume decrease
decrease pressure of system	towards *more* moles of gas	for gas: pressure decrease = volume increase
increase temperature of system	*away* from heat/ energy *exothermic* reaction is favored	extra heat/ energy must be used up
decrease temperature of system	*towards* heat/ energy *exothermic* reaction is favored	more heat/ energy needs to be produced to make up for the loss
add a catalyst	NO SHIFT	The rates of both the forward and reverse reactions are increased by the same amount.

Buffers

What is a buffer?

- A mixture of conjugate base and a weak acid
- A mixture of conjugate acid and weak base
- Must be in a ratio of 0.1 to 10

Calculating the pH of a buffer solution:

pH = pKa + log ([WB] / [WA]) -- Henderson-Hasselbach Equation

- PH is therefore = pKa ± 1

Adding an acid:

Ex. Adding 0.020 moles of HCl to 0.10 moles of AcNa, what is the

- n(HCl) will give n(H3O+) and H3O+ reacts with the base Ac- in the buffer

Rxn	HCl (aq) +	AcNa (aq) -->	NaCl (aq) +	AcH (aq)
NIE	H3O+	Ac-	AcH	H2O
Initial	0.020	0.10	0.10	NA
Change	-0.020	-0.020	+0.020	NA
End	0	0.08	0.12	NA

- Ac- / AcH = 0.08 / 0.12 = 0.67, hence we still have a buffer

Adding a base:

Ex. Consider the 1.00 L solution of C(AcH) = C (Ac-) = 0.10 M. (pKa = 4.74)
Now adding 0.020 moles of NaOH, it will give 0.020 moles of OH-

- How much AcH will be consumed?
- How much Ac- will be released?

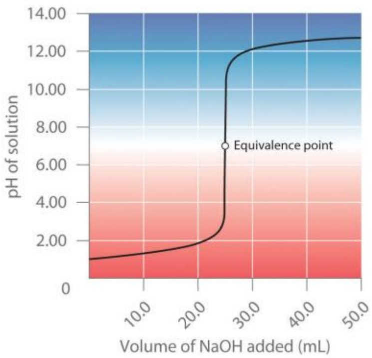
Rxn	AcH (aq) +	NaOH(aq) -->	Ac- (aq) +	H2O (aq)

NIE	AcH	OH-	Ac-	H2O
Initial	0.020	0.10	0.10	NA
Change	-0.020	-0.020	+0.020	NA
End	0	0.08	0.12	NA

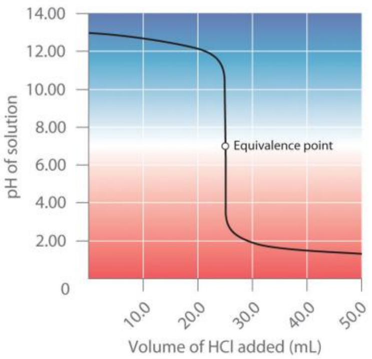
- Ratio: 0.12 / 0.08 = 1.5 , hence we still have a buffer
- Keq = (1 / Kb(Ac-)) = (1 / 5.6*10^-10) = 1.8*10^9

Titration Curves

- Equivalence point: the number of moles of acid added is equal to the number of moles of base
- End point: when the solution changes colour during a titration
- The indicator chosen should produce a colour change that is close to the equivalence point, within a pKa that is ± 1 of the pH at the equivalence point
- Finding major species
  - At 0mL of titrant: the only species is whatever you started with
  - In the buffer region: weak acid and weak base (they make up the buffer) and ions that are attached to the titrant (ex. In NaOH it would be Na+)
  - At the equivalence point: either weak acid or weak base depending on what you started with it's the opposite of what you started with (ex. If you started with HA, the major species would be A-)
  - Past the equivalence point: either weak acid or base depending on what you started with it's the opposite of what you started with and the ions attached to the titrant, plus excess H3O+/ OH- depending on if you are adding acid or base



(a) Strong acid titrated with strong base



(b) Strong base titrated with strong acid

*Know that **(a)** is a strong acid titrated with a strong base b/c:*

- pH at the equivalence point is 7
- pH started very low, as an acid which has a low pH

Know that ***(b)*** *is a strong base titrated with a strong acid b/c:*

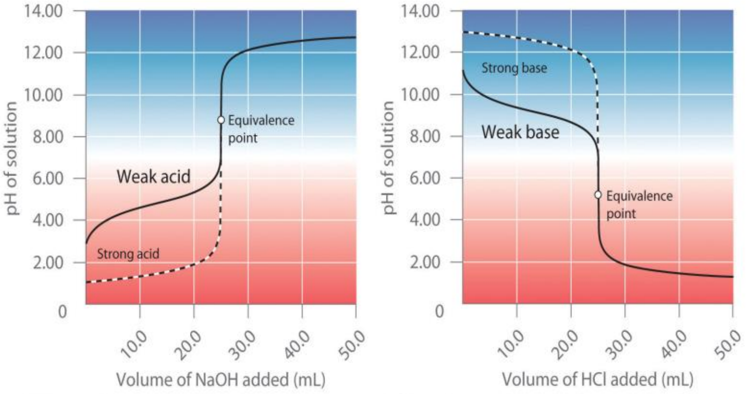
- pH at the equivalence point is 7
- the pH started very high, as a base which has a high pH level

*Know that **(a)** is a weak acid titrated with a strong base b/c:*

- equivalence point is not at 7
- the pH is slightly higher then 7 (basic properties)
- there is a tail at 0mL of volume

Know that ***(b)*** *is a weak base titrated with a strong acid b/c:*

- equivalence point is not at 7
- the pH is slightly lower then 7 (acidic properties)
- there is a tail at 0mL of volume

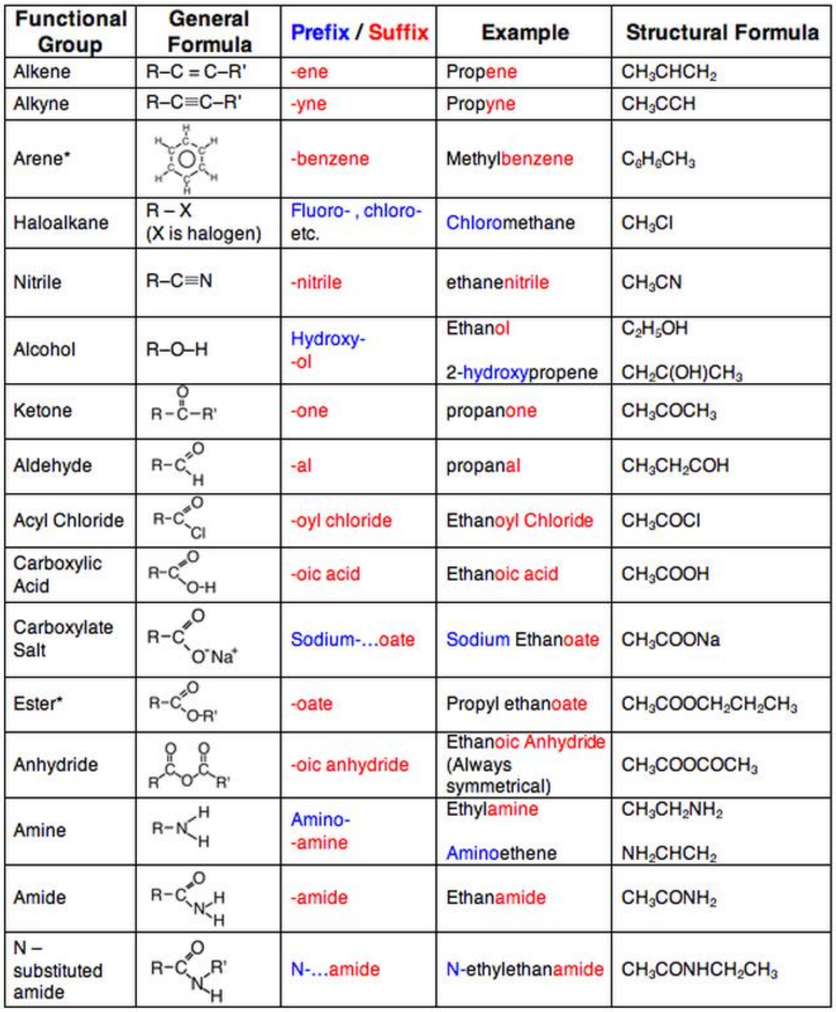


(a) Weak acid titrated with strong base **(b) Weak base titrated with strong acid**

Naming Organic Compounds

- Alkanes: single bonded long chains of carbon – they are named after their parent (longest chain) of carbons which doesn’t have to be a straight line
    - These chains may have substituents (carbons that branch off the parent chain), and they are also named after the number of carbons that are extending off the chain (1-methyl, 2-ethyl, 3-propyl, 4-butyl, etc.,)
    - There are exceptions (isopropyl, T-butyl), these substituents are names with numbers in front of them to give their location so always make sure this number is as low as possible by starting at the appropriate end
- Cycloalkanes: carbons arranged in a ring with only single bonds, in this case the substituents are not numbered unless there is more than one
- Alkenes: have double bonds and are named in the same way, with a number indicating where the double bond is
- Alkynes: have triple bonds and are names in the same way with a number indicating where the triple bond is
    - Aromatic hydrocarbons: ex. Phenol, benzene, toluene, benzoic acid – they are named according to the names above and the substituents are named according to their location: 1,2 - ‘o’/ortho; 1,3 - ‘m’/meta; 1,4 - ‘p’/para
- Organic halogen compounds (alkyl halides): hydrocarbons with halogens as substituents, they are classified as primary, secondary or tertiary based on the carbon that it is attached to (F- fluoro, Br – bromo, Cl – chloro, I – iodo)
- Ethers: carbon group-oxygen-carbon group, they are named as 2 substituents on either side of the oxygen and contain “oxy” in the middle
    - Ex. Methoxyethene – CH3OCH=CH2
- Alcohols and Phenols: hydrocarbons where an H is substituted with an OH. In order to name it, you must identify the longest chain of carbons that includes the OH group, then number the OH group, with the ending changing from ‘ane’ to an ‘anol’
    - Ex. 3-methyl-2-pentanol – CH3CH(OH)CH(CH3)CH2CH3
- Amines: derivatives of ammonia, and characterized as primary, secondary or tertiary based on the carbon that it is attached to - Acidic in nature
    - To name them, locate the nitrogen and assign a number to locate it, then change the ending from ‘e’ to ‘amine”
    - Ex. Methylamine – NH2CH3
- Aldehydes: consist of a carbonyl group (double bonded oxygen) in the end of the chain. To name them, replace the ending of ‘e’ to ‘anol’ and make sure that the carbonyl group is in the 1st location
    - Ex. Ethanal aldehyde (acetaldehyde) - CH3CHO
- Ketones: consist of a carboxyl group in the middle of the chain. To name them you must replace the ‘e’ with ‘anone’, name it based on the orientation that will give the carboxyl group the lowest number
    - Ex. Butanone – CH3COCH2CH3
- Carboxylic acid: contains a carboxylic acid group (COOH), to name them replace the ‘ane’ with an ‘anoic acid’
    - Ex. 2-ethyl-4,4-dimethylpentanoic acid – CH3C(C2H6)CH2CH(C2H5)COOH

- Ester: replaces the H with an OH of a carboxylic acid with another carbon chain, to name them it's based on the oxygen that divides the 2 carbon groups – and is named by making both carbon groups substituents and adding 'anaote' at the end
    - Ex. Butyl methanoate – CH3CH2CH2CH2OCOH
- Amides: carbonyl group attached to a nitrogen group, in order to name them you must change the 'e' to 'anamide'
    - Ex. Hexanamide – CH3CH2CH2CH2CH2CONH2



Functional Group	General Formula	Prefix / Suffix	Example	Structural Formula
Alkene	R–C = C–R'	-ene	Propene	CH_3CHCH_2
Alkyne	R–C≡C–R'	-yne	Propyne	CH_3CCH
Arene*		-benzene	Methylbenzene	$C_6H_6CH_3$
Haloalkane	R – X (X is halogen)	Fluoro- , chloro- etc.	Chloromethane	CH_3Cl
Nitrile	R–C≡N	-nitrile	ethanenitrile	CH_3CN
Alcohol	R–O–H	Hydroxy- -ol	Ethanol 2-hydroxypropene	C_2H_5OH $CH_2C(OH)CH_3$
Ketone	$R-\overset{O}{\overset{\|}{C}}-R'$	-one	propanone	CH_3COCH_3
Aldehyde	R–C(=O)H	-al	propanal	CH_3CH_2COH
Acyl Chloride	R–C(=O)Cl	-oyl chloride	Ethanoyl Chloride	CH_3COCl
Carboxylic Acid	R–C(=O)O-H	-oic acid	Ethanoic acid	CH_3COOH
Carboxylate Salt	R–C(=O)O^-Na^+	Sodium-...oate	Sodium Ethanoate	CH_3COONa
Ester*	R–C(=O)O-R'	-oate	Propyl ethanoate	$CH_3COOCH_2CH_2CH_3$
Anhydride	R–C(=O)–O–C(=O)–R'	-oic anhydride	Ethanoic Anhydride (Always symmetrical)	$CH_3COOCOCH_3$
Amine	R–N(H)H	Amino- -amine	Ethylamine Aminoethene	$CH_3CH_2NH_2$ NH_2CHCH_2
Amide	R–C(=O)N(H)H	-amide	Ethanamide	CH_3CONH_2
N – substituted amide	R–C(=O)N(R')H	N-...amide	N-ethylethanamide	$CH_3CONHCH_2CH_3$

Organic Chemistry

- Primary, secondary, tertiary carbons: determined based on the number of carbons that are attached to the carbon of interest
- Primary, secondary, tertiary hydrogens: determined based on the number of hydrogens that are attached to the carbon of interest
- Structural/ Constitutional isomers: structures that have the same chemical formula but different arrangements
- Geometric isomers: when there is a double or triple bond involved, the molecule cannot rotate freely, causing more isomers – they exist into 2 spatial arrangements (cis/trans)
    - Cis – on the same side

    - Trans – on opposite sides
- Chiral carbons: can interact with polarized light. They are most commonly characterized by having 4 different groups attached to them (they can only have 3). A chiral carbon cannot double bonded, but they can also be called enantiomers
- Intermolecular forces: decide the physical properties of the chemical compound
    - London dispersion forces: the weakest of forces, but every compound has them – based on partial charges
    - Dipole-dipole: happens when there is a large difference in electronegativity (the molecule is polar), there are strong LDFs but are not the strongest forces
    - Hydrogen bonding: happen when there is a very large difference in electronegativity, usually apparent with O, F and N bonding to carbons – these are the strongest forces
- Boiling point/water solubility and intermolecular forces: the stronger the IMFs, the higher the boiling points and the more soluble the compound is in water (like dissolves in like)
- Electrophiles: loves electrons, therefore is positive and looking for electrons to accept, often attracted to double and triple bonds
- Nucleophiles: loves the nucleus/protons, negative species that is looking to give electrons to a positive species
- Free radicals: a neutral species that has an unpaired electron

Organic Chemistry Reactions

- The only reaction with alkanes is a free radical halogenation reaction in which a halogen will replace a tertiary carbon in the presence of heat or UV light
    - However, when there is more than one carbon on the chain the halogen is most likely to replace the tertiary hydrogen than secondary or primary
- Reactions with alkenes and alkynes:
    - Electrophilic addition – an electrophile attaches itself to one of the carbons involved in the double bond (the on with least carbons attached) and then the nucleophile will attach to the other one to balance out the orbitals
    - Hydrogenation – 2 hydrogens are added to the same side of the double bond in the presence of a catalyst (ex. Nickel catalyst)
    - Polymerization – a monomer reacts with an initiator to form a long chain of identical monomers (polymer)
- Haloalkanes (alkyl halides): these hydrocarbons are prone to attack by nucleophiles b/b of the large difference in electronegativity. The halogens are replaced by a nucleophile, which causes a nucleophilic substitution
- Aromatic substitutions: the same as alkyl substitutions but aromatic compounds are extremely stable and therefore in order for this reaction to take place, it must be in the presence of a strong catalyst
- Alcohols and Phenols: remember that alcohols are very weak acids and therefore will only react with very strong bases
- Oxidation of alcohols: using potassium or sodium dichromate, this reaction converts alcohols on carbonyl groups (aldehydes or carboxylic acids). This reaction depends on whether the alcohol is primary, secondary, or tertiary
    - Primary alcohol --> (mild – Cr2O7^-2/H+) aldehyde --> carboxylic acid
    - Secondary alcohol --> (Na2Cr2O7/H+) ketone --> no further reaction

  - Tertiary alcohol --> (K2Cr2O7/ H+) no reaction
- Aldehydes and Ketones: b/c of the presence of a carbonyl group, these compounds are prone to attacks from electrophiles and nucleophiles
- Reductions: addition of H2 to form an alcohol from an aldehyde or Ketone
- Nucleophilic addition: b/c of the double bond nucleophiles are really attracted to aldehydes and ketones. This reaction will break the double bond and add another oxygen while creating an OH out of the existing one
  - Addition of water: aldehyde/ketone + H2O --> hydrate/geminal diol
  - Addition of alcohols: aldehyde/ketone + ROH --> hemiacetal
- Acid anhydride and an alcohol: the hydrogen in the OH of the alcohol reacts with the carbon attached to the oxygen in the anhydride, creating a carboxylic acid and an ester
- Direct esterification: when an acid and an alcohol combine to make an ester and water, the alcohol will split into its nucleophile and an electrophile and then remove the OH from the alcohol to make water
- Preparation of an amide: done by adding an amine and an ester together to create amide and an alcohol