

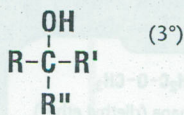
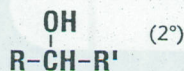
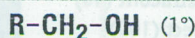
CHEMISTRY OF CARBON

- Organic chemistry is based on carbon compounds; carbon forms a wide variety of compounds with H, O, N, S, and a few other elements
- Ground state configuration of carbon is $1s^2 2s^2 2p^2$
- Easily hybridizes to produce 4 sp^3 orbitals or 3 sp^2 orbitals and 1 p orbital or 2 sp orbitals and 2 p orbitals; carbon is tetravalent
- Carbon ring and chain structures may have single, double, and triple bonds between carbon atoms
- Carbon can form 4 covalent bonds to other carbons, forming rings, branched or unbranched chains, or combinations of rings and chains
- Carbon compounds are relatively unstable to heat (i.e., decompose at elevated temperatures)

ALCOHOLS

- Alcohols are organic compounds with the hydroxyl functional group (-OH) bonded to sp^3 hybrid carbon atom
- Classified as **primary** (1°), **secondary** (2°) or **tertiary** (3°) according to classification of carbon that bears the -OH group
- Form hydrogen bonds; they have higher boiling points than ethers or hydrocarbons of the same weight
- Short-chain alcohols are soluble in water
- Methanol, propanol, and butanol are very toxic

Fermentation: $C_6H_{12}O_6 \rightarrow 2CH_3CH_2OH + 2CO_2$
(fermentation of sugar using yeast)



CH_3-OH
methanol (methyl alcohol)
BP: $64.7^\circ C$
MP: $-97^\circ C$

CH_3CH_2-OH
ethanol (ethyl alcohol)
BP: $78.3^\circ C$
MP: $-114^\circ C$

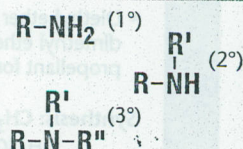
AMINES

- Amines are organic derivatives of ammonia (NH_3)
- When hydrogen atoms of ammonia are replaced by an alkyl or aryl group, the result is **primary** (1°), **secondary** (2°) or **tertiary** (3°)
- Amines are pyramidal in shape
- May form hydrogen bonds, though weaker than bonds in alcohol
- Important industrial intermediates; used in production of disinfectants, soaps, and insecticides
- Known as organic bases
- Amino acids are building blocks of proteins

Synthesis: Reduction of nitrogen groups and azides; reductive amination of aldehydes and ketones; Gabriel synthesis of 1° amines

$CH_3CH_2NH_2$ ethanamine (ethylamine)
BP: $17^\circ C$
MP: $-81^\circ C$

CH_3NH_2 methanamine (methanamine)
BP: $-6.3^\circ C$
MP: $-94^\circ C$



ORGANIC REACTIONS

ACID, BASES, ELECTROPHILES & NUCLEOPHILES

- A **Lewis acid** is an atom, molecule or ion that can accept an electron pair
- A **Brønsted-Lowry acid** donates a proton
- As **electrophiles**, they are attracted to electron-rich areas
- A **Lewis base** is an atom, molecule or ion that can donate an electron pair
- A **Brønsted-Lowry base** accepts a proton
- As **nucleophiles**, they are attracted to positive centers (nucleus)

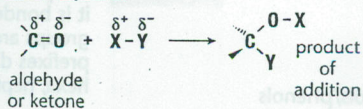
Examples: H^+ , $ZnCl_2$, NH_4^+ , SO_3 , Br^+ , carbocations

Examples: HS^- , NH_3 , OH^- , ROH , RNH_2 , N_3^- , carbanions

ADDITION

- A reaction in which 2 molecules combine to yield one molecule
- Addition frequently occurs at a double or triple bond and sometimes at small-size rings

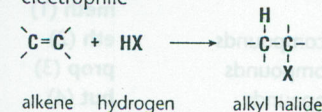
Nucleophilic



Example: Nucleophile Y bonds to carbon of the $C=O$ group; counter cation (e.g., hydrogen) bonds to oxygen

Electrophilic

- π electrons of a double bond attack an electrophile

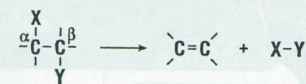


Markovnikov's Rule

- When HX is added to alkene, **H** attaches to carbon which has more Hs attached
- Does not always apply (e.g., addition of HBr with peroxide present)

ELIMINATION

- Reverse of addition; two atoms or groups are removed from a molecule



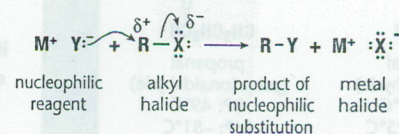
Example: A double or triple bond is formed by the loss of 2 atoms or groups of atoms

SUBSTITUTION

- A reaction in which an atom or group of atoms in a molecule or ion is replaced by another atom or group of atoms

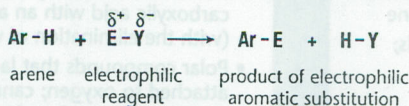
Nucleophilic Substitution

- Nucleophile Y displaces group X (e.g., a halide)



Electrophilic Substitution

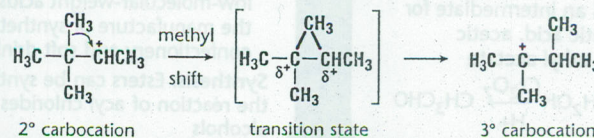
- An electrophile E displaces a hydrogen atom in the aromatic ring



REARRANGEMENT

- Reaction that converts a species to a constitutional isomer by moving bonds around

Example: Intramolecular migration of a hydride or methyl group to adjacent positively charged carbon results in a more stable carbocation



NAMING ORGANIC COMPOUNDS

- Organic compound names consist of (E) or (Z) + (R) or (S) or (-) + locants and substituents + parent chain + highest priority functional group suffix

KEY TERMS

Parent chain: Largest continuous carbon chain with the most branches • It is attached to the highest ranked functional group • All organic compounds are named after their parent chain

Substituents: Atoms or groups of atoms that replace hydrogen on the parent chain

Branches: Carbon groups that stem from the parent chain • They are named as independent units (a branch is named as a separate molecule, with its own parent chain, locants, and substituents); they end with -yl

Locants: Numbers that identify position of branches, bonds, etc. on the parent chain • Each carbon in the parent chain is numbered in order starting at end closest to highest ranked functional group • When the highest ranked functional group is an equal distance from both ends, number the carbon atoms beginning at the end nearer the first substituent

Functional groups: Molecular parts that give specific characteristics to organic compound • Compounds with similar functional groups will undergo reactions characteristic of that group

FUNCTIONAL GROUP ORDER

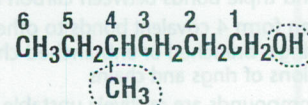
- | | |
|----------------------|------------------------------------------|
| 1 Free radicals | 10 Alcohols/phenols (equal rank), thiols |
| 2 Cationic compounds | 11 Hydroperoxides |
| 3 Anionic compounds | 12 Amines |
| 4 Acids | 13 Imines |
| 5 Acid halides | 14 Nitrogen compounds |
| 6 Anhydrides | 15 Oxygen compounds |
| 7 Nitriles | 16 Sulfur compounds |
| 8 Aldehydes | 17 Carbon compounds |
| 9 Ketones | |

NAMING ORGANIC COMPOUNDS

- Locate highest ranked functional group; usually identified by suffix added to end of parent chain prefix
- Determine parent chain (longest continuous carbon chain that contains highest ranked functional group)
 - Name is a stem determined by number of carbons
- Number carbon atoms in the parent chain, starting at end closest to the highest ranked functional group • If the branch point is same number of carbon atoms from each end, then begin numbering at end nearer second branch point
- Identify the substituents
 - Precede the name with number of carbon atom on the parent chain to which it is bonded • Multiple groups are named with prefixes di, tri, tetra, penta, hexa, hepta, octa, nona, etc.

- Identify stereochemistry of molecule
 - For (E)-(Z) system, rank groups according to Cahn-Ingold-Prelog priorities • For (R)-(S) system, rank groups according to Cahn-Ingold-Prelog priorities
- Write compound name as a word
 - Name and number of substituents are prefixes, parent chain is the stem, and the functional group is the suffix
 - Hyphens separate prefixes and commas separate numbers • Substituents are arranged in alphabetical order

Example: Name the compound



Locant identifies position of methyl group on parent chain

Prefix is the name of the substituent attached to the parent chain

4-methyl-1-hexanol

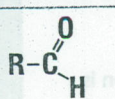
Locant identifies position of functional group on parent chain

Parent chain + suffix: -e ending in parent chain (hexane) is replaced by -ol suffix identifying an alcohol

PARENT CHAIN STEMS

meth (1)	hept (7)	tridec (13)	tetracos (24)
eth (2)	oct (8)	tetradec (14)	triacont (30)
prop (3)	non (9)	eicos (20)	hentriacont (31)
but (4)	dec (10)	heneicos (21)	tetracont (40)
pent (5)	undec (11)	docos (22)	hect (100)
hex (6)	dodec (12)	tricos (23)	

ALDEHYDES



methanal (formaldehyde)
BP: -21°C / MP: 92°C

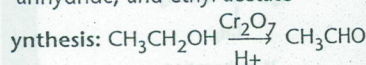
ethanal
BP: 21°C
MP: -125°C

propanal (propionaldehyde)
BP: 49°C
MP: -81°C

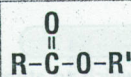
- Aldehydes have trigonal-planar geometry; carbonyl group and atoms attached to it lie in the same plane
- Easily oxidized to carboxylic acids; obtained by partial oxidation of alcohols (dehydrogenation)
- Many aldehydes have attractive odors and pleasant tastes

Formaldehyde is a colorless gas (room temperature) and dissolves in water; used as an antiseptic and pesticide, for preservation, and synthesis of polymers

Acetaldehyde is an intermediate for synthesis of acetic acid, acetic anhydride, and ethyl acetate



ESTERS



methyl ethanoate (methyl acetate)
BP: 57°C / MP: -99°C

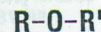
ethyl ethanoate (ethyl acetate)
BP: 77°C
MP: -82°C

ethyl benzoate (benzoic acid ethyl ester)
BP: 213°C
MP: -35°C

- Esters are formed by reacting a carboxylic acid with an alcohol (with the elimination of water)
- Polar compounds that lack a hydrogen attached to oxygen; cannot form strong hydrogen bonds with each other
- Lower solubilities in water than acids and alcohols; most esters are colorless liquids and insoluble in water
- Esters may have pleasant odors, unlike low-molecular-weight acids; used in the manufacture of synthetic flavors for confectionery and soft drink industries

Synthesis: Esters can be synthesized by the reaction of acyl chlorides with alcohols

ETHERS

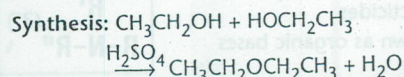


ethoxyethane (diethyl ether)
BP: 34.6°C
MP: -116°C

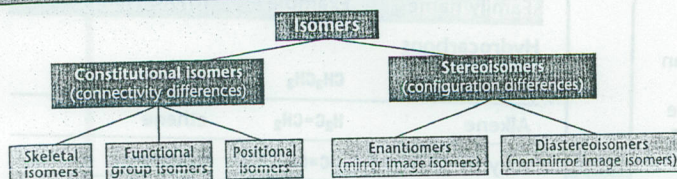
methoxyethane (ethyl methyl ether)
BP: 10.8°C
MP: -113°C

methoxymethane (dimethyl ether)
BP: -24.9°C
MP: -138°C

- Ethers are compounds in which an oxygen atom is directly bonded to two carbons, neither of which is part of a carbon-oxygen double bond
- Most notable property is comparable lack of reactivity
- Able to form hydrogen bonds with water
- Ether linkage is stable to most oxidizing and reducing agents and to action by dilute acids and alkalis; reacts with proton donors to produce oxonium salts
- Diethyl ether was used as an anesthetic; dimethyl ether (gas) is used as propellant for aerosol sprays



ISOMERISM



- Isomers are different compounds that have the same molecular formula
- Constitutional isomers** are compounds with same molecular formula that differ in the order in which atoms are bonded together
- Stereoisomers** are isomers that differ only in the arrangement of their atoms in space

ENANTIOMERS

- Enantiomers** are stereoisomers that are non-superposable mirror images of each other
- Superposability means placing one object on top of the other so that all parts of each coincide

POSITIONAL ISOMERS

- Positional isomers** are compounds which differ in the position of a given atom or group of atoms on the carbon chain

SKELETAL ISOMERS

- Skeletal isomers** differ in the order in which carbon atoms are bonded together

SKELETAL ISOMERS

- Functional group isomers differ in the type of functional group

TAUTOMERS

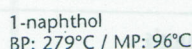
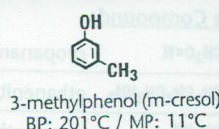
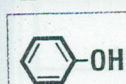
- Tautomers** are constitutional isomers in equilibrium with each other that differ in location of a hydrogen atom and a double bond; easily interconverted
- The most common are keto-enol tautomers
- Keto tautomers (e.g., aldehydes, ketones) are much more stable than enol tautomers

DIASTEREOISOMERS

- Diastereoisomers** are stereoisomers that are not mirror images and are not superposable
- Includes molecules with more than one stereocenter and *cis-trans* alkenes and cycloalkanes
- Disubstituted alkenes or cycloalkanes are designated *cis* if both substituents are on the **same side** of the carbon-carbon double bond or ring; *trans* if they are on **opposite sides**
- cis-alkene* can be named (*Z*)-alkene; *trans-alkene* can be named (*E*)-alkene

Cahn-Ingold-Prelog priorities: Scan along groups until you find a point of difference • Atom with higher atomic number has higher priority • If there is a multiple bond, then treat as 2 or 3 single bonds to atom • If isotopes, then heavier isotope has higher priority

PHENOLS

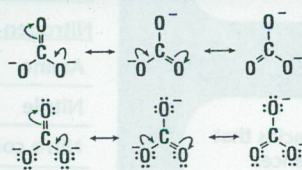


- Phenols** contain a hydroxyl group (-OH) directly bonded to a benzene ring
- More acidic than alcohols; less than carboxylic acids
- Form strong hydrogen bonds; only moderately soluble in water
- Phenol is the name of the parent compound C_6H_5OH (hydroxybenzene)

Synthesis: Chlorobenzene is heated at 350°C (under high pressure) with aqueous sodium hydroxide

Notes: Aldehydes, ketones, carboxylic acids, esters, and amides all contain the carbonyl group (carbon-oxygen double bond) but differ in what other atom or group of atoms is connected to the carbon of the carbonyl group • For some compounds, both the IUPAC and common name are given

RESONANCE



Resonance Structures of Carbonate Ion

- Resonance hybrid** is a single structure formed by a combination of contributing structures
- Resonance theory states that the actual molecule or ion is more realistically represented by a hybrid of Lewis structures (also referred to as **resonance structures** or **resonance contributors**)

HYDROCARBONS

- Hydrocarbons** are compounds that contain only carbon and hydrogen; consist of aliphatic and aromatic hydrocarbons
- Aliphatic** refers to compounds obtained from fats and oils, with a straight, branched or ring structure, that consist of alkanes, alkenes, and alkynes
- Alkanes** contain only single bonds; **alkenes** contain a carbon-carbon double bond and **alkynes** contain a carbon-carbon triple bond

ALKANES

- Alkanes** are relatively inert to many chemical reactions; C-C and C-H bonds are very strong and do not break easily
- May undergo **oxidation in air** and free radical halogenation
- Acyclic alkanes** have carbon atoms joined in a chain; includes straight chain (unbranched) and branched chain alkanes
- Cycloalkanes** have carbon atoms bonded to form a ring; nonpolar
- Carbon and hydrogen atoms possess similar electronegativity (2.5 and 2.1 on Pauling's scale)

Acyclic C_nH_{2n+2}	Cyclic C_nH_{2n}	
		<div style="display: flex; align-items: center;"> <div style="text-align: center; margin-right: 10px;"> $\begin{array}{c} H \\ \\ H-C-H \\ \\ H \end{array}$ </div> <div> methane BP: -162°C MP: -182.6°C </div> </div>
cyclohexane BP: 81°C MP: 6.5°C	cyclopentane BP: 49°C CMP: -94°C	<div style="display: flex; align-items: center;"> <div style="text-align: center; margin-right: 10px;"> $\begin{array}{c} H & H \\ & \\ H-C & -C-H \\ & \\ H & H \end{array}$ </div> <div> ethane BP: -88.2°C MP: -183°C </div> </div>

ALKENES

- Alkenes** contain carbon-carbon double bonds
- The two bonds of the C=C bond are not equivalent; the sigma (σ) bond is stronger than the pi (π) bond
- Trigonal-planar bond geometry (i.e., 2 C atoms and 4 directly bonded atoms are in the plane); there is no rotation around C=C
- Disubstituted alkenes have *cis/trans* isomers; tri- and tetra-substituted alkenes have (*E*)-(*Z*) isomers
- React with electrophilic agents (addition reactions)

Acyclic C_nH_{2n}	Cyclic C_nH_{2n-2}	
		<div style="display: flex; align-items: center;"> <div style="text-align: center; margin-right: 10px;"> $\begin{array}{c} H & H \\ C & =C \\ & \\ H & H \end{array}$ </div> <div> ethene BP: -102°C MP: -169°C </div> </div>
cyclopentene BP: 44°C MP: -98°C	cyclohexene BP: 83°C MP: -104°C	<div style="display: flex; align-items: center;"> <div style="text-align: center; margin-right: 10px;"> $\begin{array}{c} H & CH_3 \\ & \\ C & =C \\ & \\ H & H \end{array}$ </div> <div> propene BP: -47°C MP: -183°C </div> </div>

ALKYNES

- Alkynes** contain carbon-carbon triple bonds
- Linear (i.e., no possibility of *cis-trans* isomerism)
- Carbon-carbon triple bond (one sigma (σ) bond plus two pi (π) bonds) is shorter and stronger than C-C or C=C bond
- Slightly soluble in water
- Hydrogen atom of a terminal alkyne is slightly acidic
- React with electrophilic agents (addition reactions)

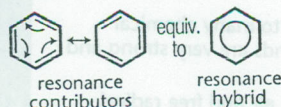
Acyclic C_nH_{2n-2}		
$H-C \equiv C-H$		ethyne (acetylene) BP: -84°C MP: -81°C
$\begin{array}{c} H \\ \\ H-C \equiv C-C-H \\ \\ H \end{array}$		propyne BP: -23°C MP: -102°C

AROMATIC COMPOUNDS

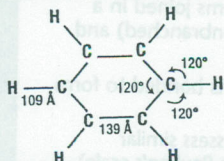
- Requirements of aromaticity: cyclic, planar, all atoms of the ring are sp^2 hybrids, + 2π electrons

BENZENES (ARENES)

Resonance Forms: Closed bonding shell of delocalized π electrons • C-C bonds are neither single nor double bonds • BP: 80°C ; MP: 5°C



Bond Lengths & Angles



DISUBSTITUTED (ORTHO, META, PARA) BENZENE DERIVATIVES

- Prefixes **1,2-**, **1,3-**, and **1,4-** (if given) can also be named **o-** (ortho-), **m-** (meta-), and **p-** (para-), respectively, to designate the positions of substituents on the ring

POLYCYCLIC AROMATIC COMPOUNDS

- Molecules that have 2 or more benzene rings fused together
- At points of fusion, 2 C atoms are common to both rings

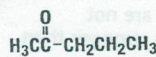
HETEROCYCLIC AROMATIC COMPOUNDS

- Ring contains element other than carbon; they are commonly encountered in biochemical systems
- Stability and chemical behavior resemble that of benzene
- Heterocyclic compounds containing nitrogen, oxygen, and sulfur are the most common

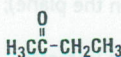
KETONES



propanone (acetone)
BP: 56.1°C / MP: -95°C

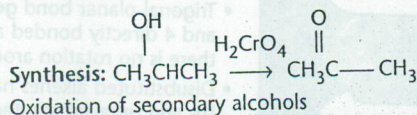


2-pentanone
BP: 102°C / MP: -78°C



butanone (methyl ethyl ketone)
BP: 80°C / MP: -86°C

- Ketones** have a trigonal-planar geometry; carbonyl group and atoms attached to it lie in the same plane
- Polar and less reactive than aldehydes
- Acetone is miscible with water in all proportions (unlike many organic solvents); volatile, highly flammable, and toxic liquid; and a good solvent for many organic substances (including varnishes, lacquers, and plastics)
- Other ketones include camphor, carvone, progesterone, and testosterone



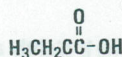
CARBOXYLIC ACIDS



methanoic acid (formic acid)
BP: 101°C / MP: 8.4°C



ethanoic acid (acetic acid)
BP: 118°C / MP: 17°C



propanoic acid (propionic acid)
BP: 141°C / MP: -21°C

- Carboxylic acids** are weak organic acids that contain COOH ; polar organic substances
- K_a for formic acid = 1.78×10^{-4} ; acetic acid = 1.74×10^{-5} ; propionic acid = 1.35×10^{-5} ; butyric acid = 1.55×10^{-5}
- Able to form strong hydrogen bonds with each other and with water; high boiling points
- Low molecular weight carboxylic acids generally show appreciable solubility in water
- Acetic acid is responsible for the sour taste of vinegar; sodium and potassium salts of long-chain carboxylic acids are major ingredients in soap

Synthesis: Oxidation of primary alcohols by potassium permanganate in basic aqueous solution

COMMON ORGANIC GROUPS

Family name	Example	IUPAC Name
Hydrocarbons		
Alkane	CH_3CH_3	ethane
Alkene	$\text{H}_2\text{C}=\text{CH}_2$	ethene
Alkyne	$\text{HC}\equiv\text{CH}$	ethyne
Diene	$\text{H}_2\text{C}=\text{CHCH}=\text{CH}_2$	1,3-butadiene
Arene		benzene

Halogen-Containing Compounds

Alkyl halide	$\text{CH}_3\text{CH}_2\text{Cl}$	chloroethane
Allyl halide	$\text{H}_2\text{C}=\text{CHCH}_2\text{Cl}$	3-chloro-1-propene

Oxygen-Containing Compounds

Alcohol	$\text{CH}_3\text{CH}_2\text{OH}$	ethanol
Phenol		phenol
Ether	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$	ethoxyethane
Epoxide		oxirane
Aldehyde	H_3CCHO	ethanal
Ketone	$\text{H}_3\text{CC(=O)CH}_3$	2-propanone
Carboxylic acid	H_3CCOOH	ethanoic acid

Carboxylic Acid Derivatives

Acyl halide	H_3CCOCl	ethanoyl chloride
Acid anhydride	$\text{H}_3\text{CCO(=O)COCH}_3$	ethanoic anhydride
Ester	$\text{H}_3\text{CCOCH}_2\text{CH}_3$	ethyl ethanoate
Amide	H_3CCNH_2	ethanamide
Dicarboxylic acid		1,2-benzenedicarboxylic acid

Nitrogen-Containing Compounds

Amine	$\text{CH}_3\text{C}\equiv\text{N}$	propanamine
Nitrile	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CN}$	ethanenitrile
Nitro compound	CH_3NO_2	nitromethane

Sulfur-Containing Compounds

Thiol	CH_3SH	methanethiol
Thioether	CH_3SCH_3	dimethyl thioether
Sulfoxide	H_3CSCH_3	dimethyl sulfoxide
Sulfone	$\text{H}_3\text{CSO}_2\text{CH}_3$	dimethyl sulfone

- A **functional group** is an atom or group of atoms in a molecule that determines the molecule's reactions
- Compounds with the same functional group that differ only by a length of an alkane chain belong to a homologous series
- Successive members of the series differ by $-\text{CH}_2-$



50395



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Quantum Numbers

- every electron in an atom has a unique quantum number
- n: Principal Quantum Number (n)**
 - labels the 2D shell the electron is in

L: Secondary Quantum Number (0...n-1)

- labels additional electron energy subshells

- orbits are actually more like elliptical-shaped orbits

ML: Magnetic Quantum Number (-L...L)

- labels direction of electron orbit (the angle that it is oriented in space)

MS: Spin Quantum Number ($-\frac{1}{2}, \frac{1}{2}$ for every value)

- describes direction electron spins on its axis
- this spin explains paramagnetism (the magnetism of individual electrons)

Lewis Theory of Bonding

- atoms/ions are stable when they have a full shell
- they are most stable when electrons are paired
- chemical bonds lead to stability
- sharing electrons between non-metals results in a covalent bond

Valence Bond Theory

- when 2 orbitals overlap to create a covalent bond, they create a new combined orbital shape
 - why orbital can have 2 electrons of opposite spin
- arranged to create maximum overlap of orbitals → lowest energy

Structure and Properties

Energy Level Diagrams

- H only gives certain frequencies of light
- energy can be calculated based on the orbital of the electron
- use **Aufbau** ("build up") process

1. draw orbitals

2. fill degenerate (equal) levels (+) then (-)

* each line holds 2 electrons

* 2 half-filled orbitals are more stable than 1 incomplete orbital

(Cr, Ag, Cu, Mo)

iso-electronic same electron config

4p	— — —
3d	— — —
4s	— — —
3p	— — —
3s	— — —
2p	— — —
2s	— — —
1s	— — —

Drawing Covalent Molecules

- determine centre element
- arrange others around it
- count total valence electrons
- draw bonds (2e- each)
- use remaining electrons to ensure every atom has 8 electrons total
- Draw [] if it is an ion

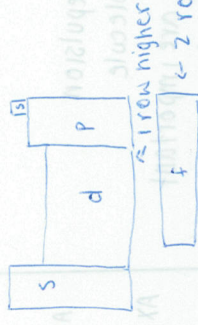
Ground State Electron Configuration

- describing elements by their electrons

[period][s, p, d, f][# filled] until all electrons are accounted for

* s^2, p^6, d^{10}, f^{14}

- shorthand [last noble gas][electrons]



← 2 rows higher than period

- unpaired electrons with the same spin can be magnetized, thus explaining **ferromagnetism** (Fe, Co, Ni in a permanent magnet)

Magnets

Ferromagnetism permanent magnet

Paramagnetism magnetic in the presence of a magnetic field

Diamagnetism oppositely magnetic in the presence of a magnetic field

Au and Cu are differently coloured than most metals because the wavelength of electrons on the surface reflect that colour of light.

- bonds between atoms are s
- 2nd/3rd bonds are π bonds

Double Bonds (sp^2)



π bonds split into top and bottom, like buns around a hot dog

Triple bonds (sp)



plus extra π

sp^3 hybrid

$\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$
s p p p p p

sp^2 hybrid

$\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$
s p p p p p

2 π bonds = 2 buns

Aromatics

- benzene



- side view: electrons

- absorbs UV light

As # of bonds increases, bond length decreases.
As # of bonds increases, bond energy increases

VSEPR

- Valence Shell Electron Pair Repulsion theory explains shape of molecule

- VSE in the central atom(s) are important

- VSE are paired in molecules / polyatomic ions

- bonded pairs and lone pairs are equal

- VSE repel each other electrostatically

- molecular shape is determined when

- VSE are max distance apart

Polarity of Molecules

- polar molecules will dissolve in water

1. draw Lewis diagram

2. calculate ΔEN of individual bonds

3. draw arrows lower(+) \rightarrow higher EN

4. add vectors

* different bonds will have different EN

Intermolecular Forces

- ionic $\Delta E = 400 - 4000 \text{ kJ/mol}$

- ex. CaCl_2

- covalent $\Delta E = 150 - 1100 \text{ kJ/mol}$

- ex. CO_2

- metallic

- $\Delta E = 150 - 1100 \text{ kJ/mol}$

- ex. CO_2

- ex. CO_2

General Formula	Bond Pairs	Lone Pairs	Total Pairs	Examples	Electron Pair Arrangement	Molecular Geometry
AX_2	2	0	2	CO_2, CS_2	linear	$\text{X} - \text{A} - \text{X}$
AX_3	3	0	3	BF_3, BH_3	trigonal planar	linear X - A - X trigonal planar
AX_4	4	0	4	$\text{CH}_4, \text{SiH}_4$	tetrahedral	tetrahedral
AX_3E	3	1	4	$\text{NH}_3, \text{PCl}_3$	tetrahedral	trigonal pyramidal
AX_2E_2	2	2	4	$\text{H}_2\text{O}, \text{OCl}_2$	tetrahedral	V-shaped
AXE_3	1	3	4	HCl, BrF	linear	tetrahedral
AX_5	5	0	5	$\text{PCl}_5, \text{SF}_6$	trigonal bipyramidal	trigonal bipyramidal
AX_4E	4	1	5	TeCl_4	trigonal bipyramidal	trigonal bipyramidal
AX_3E_2	3	2	5	BrF_3	trigonal bipyramidal	trigonal bipyramidal
AX_4E_2	4	2	6	XeF_4	square planar	square planar

Intermolecular Forces

- affects melting/boiling point, capillary action, surface tension, volatility, ion-dipole

- not really inter molecular because ion is not a molecule

$\Delta E = 40 - 500 \text{ kJ/mol}$

ex. $\text{Na}^+ \text{O}^{2-}$

Hydrogen bond

- subset of dipole-dipole

- stronger than dipole-dipole

$\Delta E = 100 - 400 \text{ kJ/mol}$

ex. H bonded to highly EN atom (ex. O, N, Cl)

- stronger than London forces, not as strong as H bond

ion-induced dipole

- a molecule that is slightly polar becomes a dipole in the presence of an ion

$\Delta E = 3 - 15 \text{ kJ/mol}$

ex. $\text{Fe}^{2+} \text{O}^{2-}$

Dipole-induced dipole

- $\Delta E = 2 - 10 \text{ kJ/mol}$

ex. H_2O and CO_2

London Force

- attraction of electrons in one molecule to positive nuclei in adjacent molecules

- exists in all molecular structures

$\Delta E = 0.05 - 0.4 \text{ kJ/mol}$

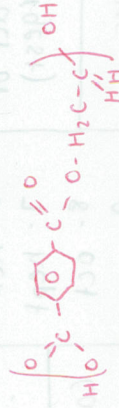
electron pairs take equatorial because they need more room

Types of Reactions

1. addition / hydration
2. elimination / dehydration / hydrolysis
3. substitution
4. oxidation
5. reduction
6. combustion

Polymers

- addition (most synthetic polymers)
- condensation (most natural polymers, some synthetic)
- made up of many repeating subunits called monomers



PET polyethylene terephthalate

Order of Functional Group Importance

1. onium ions
2. carboxylic acids
3. esters
4. amides
5. aldehydes
6. ketones
7. alcohols
8. ethers
9. amines
10. alkenes, alkynes
11. alkanes

General Catalyst Rules

- if H_2 is involved, $\text{Pd}/\text{Pt}/\text{Ni}$ is needed
- if H_2O is being added, H^+ for catalyst
- if H_2O is being eliminated, H_2SO_4 is needed to dehydrate
- if halogen is added to C , FeX_3 is needed
- if HX is added to 2° alcohol, ZnCl_2 is needed
- in oxidation (KMnO_4 , Cr_2O_7 , H_2SO_4), H^+ is needed
- in reduction, CaH_2 / LiAlH_4 / $[\text{H}]$ is needed
- in acid + base, OH^- is needed (or they will neutralize)
- in carboxylic acid + alcohol, H^+ is needed (ester lab)

Identifying Reactions

- alkene + $\text{Br}_2 \rightarrow$ colour change
- oxidation reaction \rightarrow colour change (use KMnO_4 or HCl)
- add NaOH to check acids / bases pH \rightarrow carboxylic acid + $\text{NaOH} \rightarrow$ slow change
- \rightarrow amine + $\text{NaOH} \rightarrow$ steep change



compound containing compound not clearly of mineral origin

- Hydrocarbon: Alkane, Alkene, Alkyne
- Oxygen containing: Alcohol, Ether, Ester, Carboxylic Acid, Ketone, Aldehyde
- Nitrogen containing: Amine, Amide

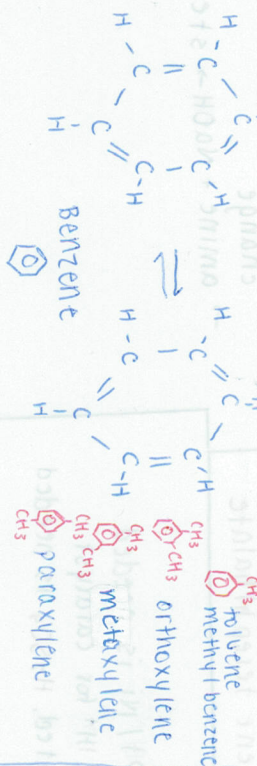
Organic Chemistry

- To name:
1. Count longest chain of carbons.
 2. Find all substituents (lowest #)
 3. list in alphabetical order or by size (smallest - largest)

Alkane - ane

- single bond
- only C-H and C-C bonds
- CH₃ methyl
- CH₂ - CH₃ ethyl
- CH₂ - CH₂ - CH₃ propyl

Aromatics (alkane) benzene



→ Xylenes

toluene methyl benzene

Alkene - ene

- 1 or more double bonds
- double bonds are point of interest because they react
- cis unnecessary when symmetrical

Alcohol - anol

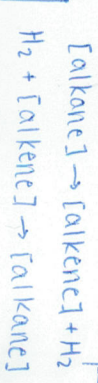
- OH bonded
- OH is acidic in organic chem because C-O bond won't ionize
- 1° alcohol OH - C - C
- 2° alcohol OH - C - C
- 3° alcohol OH - C - C
- phenol
- carboxylic acid

Ethers - oxy

- O - CH₃ methoxy bonded to 1 C
- O - CH₂ - CH₃ ethoxy bonded to 2 C
- ether - O - alkane
- [methoxy] [ethoxy] [alkane]

Reactions

Alkanes



Alkenes

- Homogeneous additions
- [alkene] + H₂ → [alkane]
- [alkene] + halogen → [alkane]
- Heterogeneous additions
- [alkene] + [acid] → [halogenated alkane]
- [alkene] + water → [alcohol]
- Markovnikov's Rule: in non-symmetrical addition to a double bond, H will attach to C with greatest # of H

Physical Properties

Alkanes, Alkenes, Alkynes

- shared electrons cause dipole
- very little attraction (low boiling point)
- longer = more energy required to boil
- stronger bonds (ex. H-bonding) = more energy required
- do not dissolve in water BUT short C chains are miscible (can dissolve in water)

Ethers

- low boiling points
- not very soluble

Aldehydes + Ketones

- soluble, but not as soluble as alcohols

LIKE

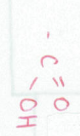
DISSOLVES

LIKE

Carbonyl - containing compounds

- > C = O carbonyl
- Aldehyde - anal
- carbonyl bonded to terminal C
- Ketone - anone / -oxo
- carbonyl bonded to non-terminal C

Carboxylic Acid - anic



Ester - anate

- derivative of carboxylic acid
- pleasant smells

[parent acid] [alkane]

[alkane] [parent acid] [anate]

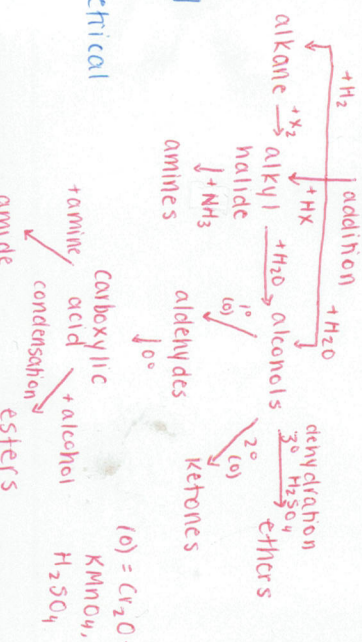
Amine - amine

- organically substituted ammonia
- H is replaced by alkane
- 1° amine N - C
- 2° amine N - C
- 3° amine N - C
- N - [short alkane] [long alkane] [amine]

Aromatics



alkenes



Metallic Bonding

Metallic Crystals

- Cu^{2+} ions are held in an array by local electrons
- if struck, the ions will **move** and electrons will fill in spots
 - deforms without changing crystal structure
 - explains conductivity as electrons move easily



Molecular Crystals

- 12 molecules form a crystal structure
- will **shatter** when hit
- ★ SiO_2 (glass) doesn't exist as a molecule, but the ratio is about 1:2
- ★ S₈ crystal can be disturbed, takes 24 h to reform



Pure Carbon Allotropes

- carbon bonded to itself makes a variety of substances
- **diamond**: 3D tetrahedral arrangements of covalent network solid
 - each C bonded to 4 other C
 - can burn like any other C
 - conducts heat very quickly
- **fullerene**: nano-sized soccer ball composed of 45, 60, etc. C atoms



- **carbon nanotubes**: fullerene that doesn't round off (like a tube)
- **graphite**: layers of sheets (flat) of sp^2 C each C bonded to 3 other C
 - conducts electricity, but is hard and has a high melting point
 - sheets are covalent network (strong), layers are London forces (weak)
 - π bonds extend over entire sheet

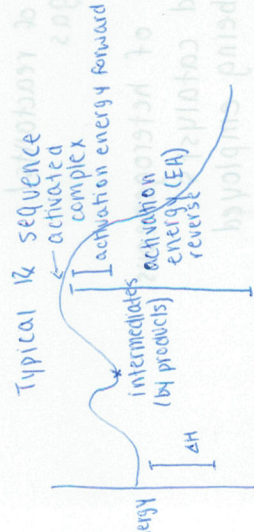


Covalent Network Crystals

- harder / higher melting point than ionic / molecular
- brittle but so hard they seldom break
- **insoluble**
- **non-conductors** of electricity
- diamond C(s), glass: quartz $\text{SiO}_2(\text{s})$, silicone carbide $\text{SiC}(\text{s})$

Calorimetry

- assuming
 - closed system
 - all heat goes into water
 - 1 ml water = 1 g
 - H_2O in product is neglig (beyond our level)
 - R_x goes to completion
- use $\Delta H = mc \Delta T$
- heat going into water = heat coming out of R_x



- activated complex

activation

reverse

EA, then

EA is

easier w/

- molecules reach **EA**, then they can continue Rx or return to reactant

- with a catalyst, EA is lower and it will have more intermediates

→ the R_4 is easier with a catalyst

Thermochemistry

- change in chemical energy
- ΔH is change in **enthalpy**
- **enthalpy**: change in general heat energy
- $\Delta H_{universe}$ is constant
- $|\Delta H_{system}| = |\Delta H_{universe}|$
- can be represented graphically, with enthalpy in the equation, or with ΔH as a separate term

- ΔH_{sol} dissolving
- ΔH_{comb} combustion
- ΔH_{vap} vaporization
- ΔH_{fr} freezing/fusion
- ΔH_{neut} neutralization
- ΔH_f formation
- ΔH° at SATP
- measured in kJ

Energy changes and Rate

Hess's Law

- any chemical R_x can be written as a series of steps \rightarrow only depends on state of reactant/product, not #

$\Delta H_{R_x} = \sum H_{R_x}$ for all steps

- you can multiply and combine steps to find ΔH for a single molecule

* whatever you find ΔH of should have a coefficient of 1 - there may be fractions

$\Delta H_{R_x} = \sum H_f^\circ \text{ products} - \sum H_f^\circ \text{ reactants}$

- use a chart of standard heats of formation $\times \#$

- subtract products from reactants

* elements in standard form have $\Delta H_f^\circ = 0$

endothermic R_x (+): absorbs heat, products have **higher T**

exothermic R_x (-): releases heat, products have **lower T**

- heat transferred to/from surroundings

$\Delta H_{system} = \Delta q_{surroundings}$

$q = mc\Delta T$ where c = specific heat capacity

$\Delta H = mc\Delta T$

- to find molar enthalpy, divide ΔH by # of moles

* remember limiting reactants!

Rate Law

- rate is proportional to product of initial concentration of reactants when they are raised to exponents



rate $\propto [A]^m [B]^n$ where m, n are 1, 2 determined by empirical data

rate = $k[A]^m [B]^n$ (slowest part of R_x)

- k is whatever it takes to equal rate \rightarrow is different for temperature, reactant, concentration, etc. in initial slope

Half Life

- 1st order R_x decompose through half-lives
- nuclear, medication, etc.

Chemical Kinetics (rate)

- rate at which product is formed / reactant is consumed

$A + B \rightarrow C + D$

average reaction rate = $\frac{\Delta \text{concentration}}{\text{time}}$

* measure whichever's conc. is easier because the ratio is consistent

Deriving Rate

- use information from trials (empirical data)
- divide trials to isolate one concentration and find the exponent
- then substitute exponents and rate to find k
- * stoichiometry does not relate to rate \rightarrow the speed you make sandwiches is unrelated to how much bread you have
- \rightarrow the exponents determine the ratios

Reaction Orders

0th order Rate = $k[A]^0$

k is in $\text{mol/L}\cdot\text{s}$

rate is not proportional to conc.

1st order Rate = $k[A]^1$

k is in s^{-1}

downwards slope because $[A]$ decreases

2nd order Rate = $k[A]^2$

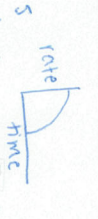
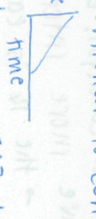
k is in $\text{L}^2/\text{mol}\cdot\text{s}$

graph is somewhat parabolic

3rd order Rate = $k[A]^3$

k is in $\frac{\text{L}^3}{\text{mol}^3\cdot\text{s}}$

steeper parabola than 2nd order \rightarrow must be calculated mathematically



Thermodynamics

4 laws

- laws are absolute; no = no but yes = maybe
- 0th law there exists an absolute 0 where matter falls apart 0 K, -273.14°C

1st law total amount of energy in the universe is constant if you include matter as a form of energy

$\Delta H_{universe} = \Delta H_{system} + \Delta H_{rest of universe}$

2nd law entropy (measure of disorder / randomness of a system) is increasing

$$S_{universe} = S_{system} + S_{row}$$

3rd law entropy of a perfectly ordered pure crystalline substance at absolute 0 is 0

Acids and Bases

Acids

- donate H^+ ions
- strong acid dissociates completely
- HCl, $HClO_3$, $HClO_4$, HBr, $HBrO_3$, $HBrO_4$, HI, HIO_3 , HIO_4 , H_2SO_4 , HNO_3 , HNO_4
- weak acids do not dissociate completely
- all other acids are weak

$$K_a = \frac{[H_3O^+][X^-]}{[HX]}$$

- H_2O is not included because concentration is constant

$$pH = -\log [H^+]$$

- use ICE table to find $[H_3O^+]$, then find pH

- 5% rule also applies here
- acids require H_2O to carry H^+ , therefore dissociation is limited by carrying capacity of water

Gibbs Free Energy

- amount of energy that is available to do work

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ \text{ where } T \text{ is in K and H is in J}$$

- $\Delta G < 0$ reaction is spontaneous forward (but needs to start)
- $\Delta G > 0$ reaction is not spontaneous

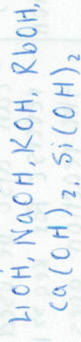
- $\Delta G = 0$ tipping point / equilibrium - when the reaction first occurs

- while ΔH of elements in standard form is 0, S is not

Bases

- accept H^+ ions

strong bases dissociate completely



- weak bases do not dissociate completely
- all other bases are weak

$$K_b = \frac{[OH^-][X]}{[XOH]}$$

$$pOH = -\log [OH^-]$$

$$pH = 14 - pOH$$

- use ICE table to find $[OH^-]$, then find pOH and pH

Dilute Strong Acids

- usually, assume the only $[H^+]$ is from acid
- in dilute strong acid or weak acid, initial $[H^+]$ is $[X \times 10^{-7}]$
- when acid is more dilute than $1.1 \times 10^{-7} M$

ΔS_{neg}

spontaneous at lower T	spontaneous at any T
spontaneous at any T	spontaneous at higher T

can react, but must have a source of energy

Conjugates

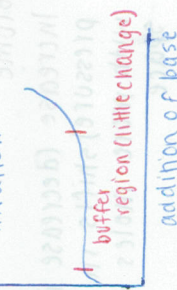
- $H_2O \rightarrow H_3O^+$ or OH^- is a conjugate pair
- the other 2 is a conjugate pair
- remember spectator ions are not included in the equation

$$K_{water} = [H^+][OH^-] = 1.0 \times 10^{-14}$$

$$K_w = [K_a][K_b] \text{ for conjugate pairs}$$

- strong acid \leftrightarrow very weak base
- weak acid \leftrightarrow weak base
- very weak acid \leftrightarrow strong base

weak acid + strong base titration



Percent Dissociation

- also known as percent ionization
- the percent of $[H^+]$ or $[DH^+]$ that dissociates
- use an ICE table
- % dissociation = $\frac{[x]}{[1 \text{ of } HX \text{ or } XOH]} \times 100\%$

Acids with $> 1 H$

- each dissociation will have a different K_a
- other than H_2SO_4 , K_{a2} doesn't matter because it is so small, it is negligible
- K_a can just be "very large" because it all dissociates
- as long as $K_a = \text{very large}$ and $[acid] < 1 \text{ mol/L}$, assume all H^+ ionizes (100% ionization)
- when doing reverse of the written reaction (product \rightarrow reactant), use K_b instead of K_a

Buffers

- used to hold pH at a set point
- commercial products to control
- ex: soaps, beverages, candy
- weak acid + salt of weak acid
- weak base + salt of weak base
- use ICE table to calculate pH
- initial $[X^-]$ is affected by the salt
- $-\log [H^+] = -\log K_a + \log \frac{[X^-]}{[HX]}$ for weak acids/bases

dynamic Equilibrium

- reactions are reversible (forward and reverse reaction)
- occurs when
 - reversible process, rate of opposing changes are equal
 - observable properties are constant (no changes)
- closed system
- can be approached from either direction

$$\text{rate}_{\text{forward}} = \text{rate}_{\text{reverse}}$$

- * in no case is the reacting species completely consumed

K_{eq} equilibrium constant (unitless)

$$K_{eq} = \frac{[C]^c [D]^d}{[A]^a [B]^b} \quad \frac{\text{product}}{\text{reactant}}$$

where $aA + bB \rightarrow cC + dD$
in direction it is written, not direction it is going

- * solids do not affect K_{eq} because they do not change concentration
- * coefficients = exponents

Le Chatelier's Principle

when system is disturbed, equilibrium shifts in direction to counteract it

Concentration

- increase shifts to opposite of the side added to reach equilibrium
- Decrease shifts to same direction of side taken away to reach equilibrium

* catalysts do not change direction, but increase rate

* inert gases do not react, affect concentration of product/reactant,

Equilibrium

$K_{eq} \gg 1$ prod \gg react; reaction proceeds towards completion

$K_{eq} = 1$ prod = react; reaction proceeds towards partial completion

$K_{eq} \ll 1$ prod \ll react; barely reactive

ICE Tables

- initial, change, Equilibrium
- where $x = \Delta$ in conc.
- sub values into K_{eq} equation and solve
- * remember coefficient in equation

* written in moles/L

Temperature

- endothermic ($R + \text{energy} \rightleftharpoons P$)
- exothermic ($R \rightleftharpoons P + \text{energy}$)
- increase shifts in direction that doesn't produce energy to "cool"

Decrease shifts in direction that produces energy to "warm"

Volume

increase (decrease in pressure) shifts in direction with more moles to fill space

Decrease (increase in pressure) shifts in direction with less moles to fit space

* things can have no effect even when conc., T, v are changed

K_{eq} Manipulation

$K_{new} = 1/K_{old}$ when a reaction is reversed

$K_{new} = (K_{old})^n$ if a reaction is multiplied by n

$K_{new} = K_1 K_2$ if 2 reactions are added together

$K_P = K_{eq} (RT)^{\Delta n_{\text{gas}}}$ for gas phase equilibria

Approximations

- when $K_{eq} \ll 1$ or $K_{eq} \gg 1$, approximations can be used to simplify calculations

- 5% Rule: $c - x = c$
→ ignore the x because it is $< 5\%$ of c

- can also be used in reverse for $K_{eq} \gg 1$ as the reaction goes to completion

Reaction Quotient (Q)

- same formula as K_{eq}

- calculated using concentration at any given point (not equilibrium)

$Q > K$ [prod] decreases, [react] increase reverse direction

$Q = K$ [prod] no change, [react] no change at equilibrium

$Q < K$ [prod] increases, [react] decrease forward direction

Solubility

- saturated solution: the max amount of solute is dissolved in the solvent for that temperature

- K_{sp} K of solubility product

- solids do not count in x equation. ∴ use solid \rightleftharpoons solutes in $K_{sp} = [A][B]$



- use ICE table to solve for x

Trial Ion Product

- use Q to discover if there is a precipitate

$Q < K_{sp}$ unsaturated solution $Q > K_{sp}$ supersaturated solution (precipitate)

- when using Q to predict precipitate of a reaction:

1. write equation and find potential precipitate
2. find conc. of individual solutions
3. find conc. when solutions are mixed together $[] = M \cdot \frac{\text{initial}}{\text{total}}$
4. calculate Q
5. compare to K_{sp} that is given

Common Ion Effect

- when equilibrium exists in a solution involving ions, it can be shifted by adding any compound that adds a common ion or that reacts with one of the ions already in solution

* the concentration of one substance will never be 0 as they are factors

Electrochemistry

- reactions that involve **transfer** of electrons from one element to another

oxidation: losing electrons

reduction: gaining electrons

* oxidation does not always require oxygen

LEO says GER

- organic oxidation agents:



Electricity

1 amp = 1 coulomb/s

1 C = 6.24×10^{18} e⁻

1 e⁻ = 1.602×10^{-19} C

Farraday's constant:

$F = 9.65 \times 10^4$ C/mol

$q = It$ where q = charge in C

I = current in amp

t = time in s

$n_e = \frac{q}{F}$ where n_e is electric charge in moles

$$n_e = \frac{It}{F}$$

* in electroplating, multiply # of moles by oxidation # based on how many e⁻ are released

Oxidation Numbers

- every element in a chemical compound can be assigned a number based on electrons

- all atoms in an element are 0

- H in all compounds is 0
→ but hydrides are -1

when H is lost element

- 0 in all compounds is -2
→ but peroxides are -1

- alkali metals are +1

- alkaline earth metals are +2

- halogens are -1

- total of polyatomic ions is charge on ion

Galvanic Cell

- produces electricity

- electricity flows **anode** → **cathode**

- strongest oxidizing agent is reduced at cathode

- strongest reducing agent is oxidized at anode

- standard cell has concentration of 1 mol/L

- requires porous barrier or salt bridge

Electrochemistry

- can be used to balance rxn

1. mark **oxidation #** of each element
2. connect **oxidations** and note e⁻ change

3. connect **reductions** and note e⁻ change

4. find **LCM** of e⁻ change

5. **balance** to find **LCM**

6. add H⁺ or H₂O to balance O and H

- (for bases: add OH⁻ on both sides to balance # of H⁺ combine OH⁻ and H⁺ to make H₂O)

7. check **overall charge**

Half-Reactions

- oxidation and reduction reactions are separated, balanced separately and recombined

1. separate into 2 equations:

oxidation and **reduction**

2. balance **all elements** that are not H and O

3. balance **O** by adding **H₂O**

4. balance **H** by adding **H⁺**

(for bases: add OH⁻ to both sides to balance # of H⁺

combine OH⁻ and H⁺ to make H₂O)

5. balance **charge** by adding e⁻

6. **cancel** out anything that is the same on both sides

7. find **LCM** of e⁻ in both equations and **combine** both equations

