# Unit 1: Organic Chemistry

#### **Hydrocarbons**

Hydrocarbon:

Things to know:

- Number of carbons give base of name
- Follow rules
- $\bullet \quad C_n H_{2n+2}$
- Number of carbons:

meth, eth, prop, but, pent, hex, hept, oct, non, dec

Prefix + root + suffix

Numbers location

Di, tri

Alkane: single bonded hydrocarbon Alkene: double bonded hydrocarbon Alkyne: triple bonded hydrocarbon Complete structural diagram Condensed Structural diagram Line Structural diagram

#### Rules:

- 1. Prefix, branch position(s), name of branches
- 2. Root number of carbon atoms on parent chain
- 3. Longest chain of carbons atoms is the parent
- 4. Parent chain must include double/triple bonds
- 5. Start the parent chain closest to a branch
- 6. Name each branch and its location
- 7. Sort branches in alphabetical order
- If > 1 of the same branch adds multiplying prefix (di, tri ..)
- 9. Comma between numbers, hyphen between numbers/letters

#### Branches:

-F	fluoro
-Br	bromo
-Cl	chloro
-1	iodo
-OH	hydroxy
-NO <sub>2</sub>	nitro
-NH <sub>2</sub>	amino
-COOH	carboxy

# Aliphatics, Aromatics, Cyclic Compounds

Carbons join in a ring shape are Cyclic Compounds, prefix (Cyclo)

Alkyl branches:

Isopropyl <mark>Y form branch</mark>	$\mathbf{x}$
N-butyl Butyl branch attached at <mark>position</mark> <mark>1</mark>	~~~
sec-butyl 2nd grade attached at <mark>position</mark> <mark>2</mark>	~~~
tert-butyl 3rd grade <mark>+ shape</mark>	$\rightarrow$

Benzene:  $C_6H_6$ , electrons are shared, planar ring

Branch	Location
Para (p)"across"	1,4
Meta (m)"middle"	1,3
Ortho (o)"next door"	1,2

When benzene is a branch it is phenyl

#### Isomers

When a molecule has different possible structures it is called an isomer <u>Constitutional Isomers</u> are molecules that have different bonding with the same formula. Ex. C7H16 can be shown: 2-methylhexane / 2,4-dimethylpentane



<u>Stereoisomers:</u> molecules that have same bonds but different arrangements Cis-trans are possible for alkenes that posses two branches



Cis: Hydrogens on same sides



Trans: Hydrogens on opposite sides Complex Organic Compounds:

Alcohols, Ethers, Aldehydes, Ketones, Carboxylic Acids, Esters, Amines, Amides <u>LISTED IN ORDER OF NAMING</u> <u>IMPORTANCE HIGHEST TO LOWEST:</u>

Carboxylic Acids: A hydrocarbon with a carboxyl group (C(=O)OH) attached to an alkyl group Name parent Replace -e with <mark>-oic acid</mark> The carboxyl group always given position 1



Esters: A hydrocarbon with a double bonded oxygen and a single bonded oxygen (O-C=O) attached to two alkyl groups 1.Longest parent chain with C=O group 2.Replace -e with -oate

3.Put space between alkyl group name attached and the parent chain



Amides: A hydrocarbon with a bonded nitrogen with a double bonded oxygen (N-C=O) attached to 1 to 3 alkyl groups Longest that contains C=O is parent Replace -e with -amide

1 degree, no alkyl groups attached to the nitrogen

2 degree, 1 alkyl groups attached to the nitrogen

3 degree, 2 alkyl groups attached to the nitrogen



Aldehydes: A hydrocarbon with double bonded oxygen (=O), single bonded hydrogen (H) Name parent with C=O group, position 1 no numbers

Replace -e with -al



Ketones: A hydrocarbon with a double bonded oxygen (C=O) attached to two alkyl groups

Longest chain with C=O os parent Replace -e with -one and is needed, di, tri Number if more than 4 carbons



<u>Alcohols:</u> A hydrocarbon with a main hydroxyl (OH) branch 1.Longest chain with <mark>OH</mark> group 2. Replace -e with <mark>-ol</mark>

3. Add **number** if needed and multiplying prefix to -ol



<u>Amines</u>: A hydrocarbon with a bonded nitrogen (N) attached to 1 to 3 alkyl groups 1.Longest attached to nitrogen (-N) 2.Replace -e with -amine

3.N- instead of number locations is gives N to branches on the nitrogen



Ethers: A hydrocarbon with an oxygen (-O-) between two alkyl groups 1.Longest chain is parent 2.Second alkyl group is branch but replace -yl with -oxy, give position number 3.Alkoxy group + parent alkane



Akenes Alkynes Alkyl Halides Alkanes (lowest priority)

### BOTTOM OF ORDER OF IMPORTANCE

Types of Reactions: Combustion, Addition, Substitution, Elimination, Condensation, Hydrolysis, Oxidation, Reduction, Synthesis and Esterification

Markovinkov's Rule: Hydrogen will bond with a carbon with the most hydrogens Combustion: All hydrocarbons undergo combustion in the presence of oxygen  $C_nH_{2n+2} + O_2 \rightarrow CO_2 + H_2O$  Addition: Breaks double/triple bonds and adds atoms to them  $CH_2CHCH_2CH_3 + H_2 \rightarrow CH_3CH_2CH_2CH_3$ Substitution: Hydrogen atom being replaced with a halide atom (needs catalyst)  $CH_3CH_2CH_3 + Cl_2 \rightarrow CH_3CH(CI)CH_3 + HCI$ Elimination: A double/triple bond formed out of the removal of atoms  $CH_3CH(CI)CH_3 + NaOH \rightarrow CH_3CHCH_2 +$  $NaCI + H_2O$ Condensation: make water from synthesis of amides Carboxylic acid + ammonia  $\rightarrow$  amide

 $CH_3COOH + NH_3 \rightarrow CH_3ONH_2 + H_2O$ 

#### Hydrolysis:

Amines: split water to from carboxylic and amine from an acid/base and amide  $CH_3ONH_2 + H_2O \rightarrow CH_3COOH + NH_3$ Esters: split water with ester into carboxylic acid and alcohol  $CH_3(O)OCH_3 + H_2O \rightarrow HCOOH + CH_3OH$ Oxidation: Carbon forms more bonds with oxygen and less with hydrogen using an oxidizing agent 1 degree Alcohol  $\rightarrow$  aldehyde  $CH_3CH_2OH$  [O] $\rightarrow CH_3COH$ 2 degree Alcohol  $\rightarrow$  ketone  $CH_3CH(OH)CH_3[O] \rightarrow CH_3COCH_3$ Aldehyde  $\rightarrow$  carboxylic acid  $CH_3COH + H_2O \quad [O] \rightarrow CH_3CH_2OH$ Reduction: Aldehyde reduced with hydrogen gas to form 1 degree alcohols Ketones reduced with hydrogen gas to form 2 degree alcohols Aldehyde [H]→1 degree Alcohol  $CH_3CH_2OH [H] \rightarrow CH_3COH$ Ketone [H]→2 degree Alcohol  $CH_3COCH_3[H] \rightarrow CH_3CH(OH)CH_3$ Synthesis: Halide reacts with ammonia to synthesize an amine Primary amine  $CH_3CI + NH_3 \rightarrow CH_3NH_2 + HCI$ Secondary amine  $CH_3CI + NH_2CH_3 \rightarrow CH_3NHCH_3 + HCI$ 

Tertiary amine

CH<sub>3</sub>CI + CH<sub>3</sub>NHCH<sub>3</sub>→CH<sub>3</sub>N(CH<sub>3</sub>)CH<sub>3</sub> + HCI Esterification: Carboxylic acid and alcohol react to form water and an ester HCOOH + CH<sub>3</sub>OH → CH<sub>3</sub>(O)OCH<sub>3</sub> + H<sub>2</sub>O **Properties of Organic Compounds** Solubility: affected by polarity nonpolar molecule will be insoluble in H<sub>2</sub>O Boiling point: affected by types and amount of IMF and shape. L.D. forces are in all atoms. More atoms higher boiling point b/c more IMF. Polar and dipole-dipole have higher boiling points. Sate: more atoms more solid organic

compounds get

# Unit 2: Structures and Properties of Matter

Atomic History (Models of the atom) Aristotle only four elements: earth, air, fire and water Democritus (300 B.C): atoms are made of tiny, indivisible things Dalton's Atomic Theory: All matter made up of tiny particles ("atoms") Thomson Model of the Atom: electrons could be emitted from matter Robert Millikan (1909): calculate relative charge and mass of the electron Ernest Rutherford (1911): discovered atom is mostly empty space James Chadwick (1932): Proved the existence of the neutron. Neils Bohr: - The Planetary Model Max Planck (1900): Quantum Hypothesis made to explain observations. **Einstein (1905):** the energy of the photon is transferred to the electron Quantum Model of the Atom (quantum numbers) Principal (n) - Values from (1,2,3...), size and energy of orbital, n is number of types of orbitals, n<sup>2</sup> number of orbital in ground state

<u>Secondary (/)</u> 0 to n-1, shape of orbital, /=0 (s) sharp, /=1 (p) principal

Magnetic (m<sub>l</sub>) / to -/, orientation of orbital, number of suborbitals

<u>Spin (m<sub>s</sub>)</u> direct and magnitude of electrons axial spin, 2 possible spins, 2 electrons per orbital

## **Energy Level Diagrams**

n values increase upwards as energy increases, orbitals distance gets smaller further up, overlap at high

#### Aufbau Principle:

Energy level must be filled before moving up next level

#### Pauli Exclusion Principle:

No 2 e<sup>-</sup> in an atom can have 4 quantum numbers, on 2 e<sup>-</sup> can exist per orbital Hund's Rule:

1 e<sup>-</sup> is placed in each suborbital



#### **Electron Configuration**



# n / #

n = energy level

/= sublevel

- # = number of electrons
- Iron electron configuration:

1s2 2s2 2p6 3s2 3p6 4s2 3d6

Abbreviated form is from last noble gas [Ar] 4s2 3d6

# **Chemical Bonding**

lonic Compounds: made of ionic bonds, usually between metals and nonmetals, bonded in a crystal lattice structure,  $\Delta EN \ge 1.7$ 

<u>Molecular Compounds:</u> covalent bonds between 2 nonmetals,  $\Delta EN = 0$  to 0.5 is nonpolar covalent /  $\Delta EN = 0.5$  to 1.7 is polar covalent

Simple covalent: each atom shares 1 e<sup>-</sup> for bonding

<u>Coordinate covalent:</u> 1 atom shares 2 e<sup>-</sup> for bonding

# Lewis Structures (including resonance)

Steps:

- 1. Find number of electrons for every atom and sum them
- 2. Draw central atom (usually only 1 atom is central)
- Draw single bonds first (take away 2e<sup>-</sup> for every bond)
- 4. Put remaining e<sup>-</sup> on the outer atom to fill their octets
- 5. Put leftover e<sup>-</sup> on middle atom in pairs
- 6. If central atom does not follow octet rule add double/triple bonds by changing around electrons
- 7. Check for resonance structures
- 8. Find vector of molecules by making the atom with the highest  $\Delta$ EN the negative side and the opposite the positive side
- 9. Draw vectors if molecule is polar and dipoles
- 10. Put square brackets around the structure if it is an ion and a charge number

Resonance: when a lewis structure can be changed while not affecting its properties





# **Formal Charge**

**F.C.** = number of valence e<sup>-</sup> - number of unbonded e<sup>-</sup> - number of bonds Structure that has the most zeros is best Overall number of valence should be equal to zero or if an ion its charge

-O: 6 - 6 - 1 = -1 =O: 6 - 4 - 2 = 0 N: 5 - 0 - 4 = +1

#### Molecule Polarity and VSEPR Theory

Bond Polarity: disturbing of e<sup>-</sup>across single bond

Molecular polarity: is polarity of sum of all bonds in a molecule

Polar molecule: unequal e<sup>-</sup> arrangement producing a negative charge at one end and a positive charge at the other

<u>Non-polar molecule</u>: equal e<sup>-</sup> arrangement producing no net charge

The type of bond and the location of the bond in the molecule determines if it is polar/non-polar

Get ∆EN

Example:

N: 3.04

O: 3.44

 $\Delta EN = 3.44 - 3.04 = 0.40$ 

: bond nonpolar and molecule is nonpolar

VSEPR SUMMARY

Number of electron pairs around central atom			Full description of the molecule				
BONOING (E)	LONE (E)	Example	Bond angles "	Geometry of Electron Pairs	Geometry of Atoms	3D Shape	Type
2	0	BeCly	180	Linear	Linear	00	AB <sub>2</sub>
3	0	BF3	120	Trigonal planar	Trigonal Planar	<u>,</u>	AB <sub>3</sub>
2	1	SO2	Slightly less than 120	Trigonal planar	Bent or V Shaped	$\overline{\mathbf{A}}$	AB <sub>2</sub> E
4	0	CH4	109.5	Tetrahedral	Tetrahedral	~	AB.
3	1	NH <sub>3</sub>	107.5	Tetrahedral	Trigonal Pyramidal	0%	ABJE
2	2	H <sub>2</sub> O	104.5	Tetrahedral	Bent or V Shaped	~~	AB <sub>2</sub> E
5	0	PCIs	120 in plane. 90 perpendicular to plane	Trigonal bipyramidal	Trigonal Bipyramidal	200	ABs
4	1	SF4	Complex	Trigonal bipyramid	Seesaw	000	AB4E
3	2	CIFs	Approx. 90	Trigonal bipyramidal	T-Shaped	÷	AB <sub>3</sub> E,
2	з	XeF2	180	Trigonal bipyramid	Linear	÷.	AB <sub>2</sub> E
6	0	SF6	90	Octahedral	Octahedral		ABe
5	1	BrFs	Approx. 90	Octahedral	Square Pyramidal		AB₀E
4	2	XeF4	90	Octahedral	Square Planar	a	AB4E

# trigonal planar for NO<sub>3</sub>-

Valence Shell Electron Pair Repulsion

Determines structure around atom by minimizing repulsive force Bonded and unbonded e<sup>-</sup> repel each other far away to minimize repulsive force Lone pair e<sup>-</sup> pushes bonding pairs of e<sup>-</sup> together changing angles because they are

more repulsive

Treat multiple bonds as single bonds

A = middle atom

X = surrounding atoms

- $\varepsilon$  = lone pair e<sup>-</sup>
- $\therefore$  AX<sub>3</sub> for NO<sub>3</sub><sup>-</sup>

# Hybridization

Orbital hybridization can explain the shape of the molecule

Carbon as example can make 4 bonds because it promotes one e<sup>-</sup> from 2s to the 2p orbital

Hybrid orbitals only exist when bonding occurs to form a molecule, not in atoms

Sigma bonds: occurs when there is end to end overlap of orbitals - a single covalent bond

<u>Pi bonds:</u> occurs when there is overlap above and below the plane of the bond, "sideways", overlap of p orbitals - o double or triple bond contains a pi component bond



## Unit 3: Energy Changes & Rates of Reactions

### Thermochemistry

Thermochemistry means study of change in energy

Energy measured in joules (J) is the ability to do work

<u>Potential Energy</u> is the energy of something because of its position or composition

<u>Kinetic Energy</u> is the energy of an object because of its motion

Thermal energy is the total amount of kinetic and potential energy

Heat is the transfer of thermal energy from object to object

Temperature is a measure of the average kinetic energy

The Law of Conservation of Energy: energy cannot be created or destroyed, it only can be converted

A group of reactants and products being studied is a chemical system

Anything that is not the system is the surroundings

An <u>open system</u> is a system open for energy and matter to move in and out freely A <u>closed system</u> is a system where energy can enter/leave the system but not matter An <u>isolated system</u> is an ideal system where matter or energy cannot move in or out An <u>exothermic</u> chemical reaction is when energy is released An <u>endothermic</u> chemical reaction is one in which energy is absorbed

### Heat Capacity (Q) and Calorimetry

Specific heat capacity (c) is the amount of thermal energy need to increase the temperature of 1g of a chemical by 1 °C <u>Specific heat capacity</u> depends on state and substance type

<u>Calorimetry</u> is the process of recording the thermal energy change of a substance Calorimetry calculations depend on 4 assumptions:

- Any thermal energy moved from the calorimeter to the outside is not counted
- 2. Any thermal energy absorbed by the calorimeter is not counted
- All dilute, aqueous solutions have the same density (1.00g/mL) as water
- Diluted, aqueous solutions have the same specific heat capacity (4.184 J/(g•°C)) as water

# <mark>Q = mc∆T</mark>

**Q** is the total amount of thermal energy/ heat

m is the mass in grams

c is the specific heat capacity in J/(g•⁰C) ΔT is the temperature change of substance

#### <u>T<sub>f</sub> -T</u>j Q<sub>svstem</sub> = - Q<sub>surroundings</sub>

An increase in the temperature of the water indicates an exothermic rxn, whereas a decrease in the temperature of the water indicates an endothermic rxn 300g of an unknown metal at 400°C is dropped into 500mL of water at 21.5°C. The water is heated up to 74.6°C, what is the heat capacity of the metal?  $Q=(500g)(4.184 J/g^{\circ}C)(53.1^{\circ}C)$  $Q_{water}=111,085.2 J$  $Q_{meta}I=-111,085.2 J$  $c=-111,085.2J / (300g)(-840.4^{\circ}C)$  c=0.44060447 J/g°C c=0.4406 J/g°C

# Enthalpy (ΔH)

Enthalpy (H): is total amount o f thermal energy in a system ro substance Total kinetic energy + total potential energy = thermal energy

Cannot measure enthalpy of a system directly

Enthalpy change ( $\Delta$ H) is the energy transferred to or from the surroundings during a chemical or physical change

# $\Delta H_{system} = +/-[Q_{surroundings}]$

<u>Endothermic</u> is when  $\Delta H$  is negative <u>Exothermic</u> is when  $\Delta H$  is positive Signs are always required for enthalpy Molar enthalpy change ( $\Delta Hx$ ) is the enthalpy change of 1 mole of a substance, units kJ/mol

4 way to show enthalpy change:

Thermochemical equations with energy terms:  $1/2 O2_{(g)} + H2_{(g)} \rightarrow H2O_{(l)} + 285.8 \text{ kJ}$ Thermochemical equations with  $\Delta H$ :

 $\begin{array}{l} 1/2 \ O2_{(g)} + H2_{(g)} \rightarrow H2O_{(l)} \\ \Delta H = -285.8 \ \text{kJ} \\ \text{Molar Enthalpy } (\Delta \text{Hx}): \\ 1/2 \ O2_{(g)} + H2_{(g)} \rightarrow H2O_{(l)} \\ \Delta \text{Hx} = -285.8 \ \text{kJ/mol} \\ \text{Potential energy Diagrams:} \end{array}$ 

#### <mark>∆H=(n)(∆Hx)</mark>

x = type of change

#### Hess's Law

Hess's La: enthalpy change ( $\Delta$ H) is determined by initial and final conditions of a system

#### $\Delta H_{\text{reaction}} = \sum \Delta H_{\text{steps}}$

Hess's law is used when the reaction target is too slow, too fast, too dangerous, or not possible to do in a calorimeter. Reverse rxn(flip) must also flip  $\Delta H$ Ensure rxn is balanced to mach target (multiply)

#### Example equation:

$2C(s, \text{ graphite}) + 2O_2(\overline{g}) \rightarrow 2CO_2(\overline{g})$	$\triangle H = -787.0 \text{ kJ}$
$\mathrm{H}_{2}(g) + \frac{1}{2}\mathrm{O}_{2}(g) \rightarrow \mathrm{H}_{2}\mathrm{O}(t)$	$\bigtriangleup \mathrm{H} = -285.8~\mathrm{kJ}$
$\underline{2C\Theta_2(g)} + \underline{H_2\Theta(t)} \rightarrow C_2H_2(g) + \frac{5}{2}Q_2(g)$	riangle H = 1301.1  kJ
$2C(s, \text{ graphite}) + H_2(g) \rightarrow C_2H_2(g)$	$\triangle H = 228.3 \text{ kJ}$

Example chart:



# Standard Enthalpy of Formation (ΔH°f)

<u>Standard molar enthalpy:</u> is the change in enthalpy ( $\Delta H^{\circ}f$ ) when 1 mol is formed directly from its elements

<u>Molar quantity:</u> amount of energy required to form 1 mole of a substance from its elements in their standard states

 $\Delta$ Hf compounds can be found in a table  $\Delta$ H =  $\sum[(n)(\Delta$ Hf Products)] -  $\sum[(n)(\Delta$ Hf Reactants)]

# Entropy (ΔS) (Spontaneous Change)

Entropy (S) is the amount of chaos of a system (higher entropy means more chaos)

# $\Delta S = \sum [(n)(\Delta S \operatorname{Products})] - \sum [(n)(\Delta S \operatorname{Products})]$

#### Reactants)]

- 1. ∆S > 0
- 2. Increase in state
- Number of moles products > reactants

# Gibb's Free Energy (ΔG)

#### <u>ΔG = ΔΗ -ΤΔS</u>

If  $\Delta G$  is + not spontaneous If  $\Delta G$  is - is spontaneous Ideal values for a spontaneous reaction:  $\Delta H = -$  (exothermic)

# $\Delta S = + (high entropy)$

# <u>∆G = -</u>

Example:

ΔS = +90Kj ΔH = +340Kj T=300K

 $\Delta G = 340-(300)(90)$  $\Delta G = -26660$  $\therefore$  rxn is spontaneous

# Chemical Reaction Rates (Collision Theory and Factors that Affect Reaction Rates)

Reaction Rate: is the speed at which a reaction occurs

<u>Collision theory:</u> chemical reactions can occur only if reactants collide with the right orientation and enough energy to break and form bonds

Activation Energy: the minimum energy for a collision to be effective

5 factors that can cause this increase:

- Chemical nature of the reactants
- Concentration
- Surface Area
- Temperature
- Catalyst

<u>Average Reaction Rate:</u> is the change  $\Delta$  in reactant or product concentration over a given time interval

<u>Rate determining step:</u> slowest elementary step

The units for average reaction rate are mol/L•s

Reaction Order	K units
0	mol/L x s
1	1/s or s-1
2	L/mol x s
3	L²/mol² x s

# Rate Law

Rate – measuring the change in [reactant] or [product] over time.

k is the Rate Constant

x and y are determined experimentally, and do not depend on stoichiometric

# <u>rate = K[A]<sup>x</sup>[B]<sup>v</sup>[C]<sup>z</sup></u>

coefficients from balanced equation total order: sum of the exponents <u>Average Reaction Rate:</u> is the change  $\Delta$  in reactant or product concentration over a given time interval

- 1. Using at least 3 sets of data for the reaction
- 2. Write out the rate law equation with the reactants used
- 3. Find 2 experiments where 1 of the reactants is constant but the other changes.
- 4. Compare the rates and the concentrations to solve for the exponent
- 5. Find two data points where the 2nd of the reactant remains constant and the other changes
- 6. Compare the rates and the concentrations to solve for the exponent
- Using one set of experimental data, and the values for exponent, solve for k
- Units of k can be found by keeping them in the equation or the table for K units

# Unit 4: Chemical Systems and Equilibrium

# Dynamic Equilibrium

Most reactions one-way reactions Most reactions are mixture of both reactants and products

Forward rate: rate at which the products are formed.

Reverse rate: rate at which the reactants are re-formed.

Reaction almost never stops always in a state of equilibrium (back and forth)

Equilibrium: is when f<sub>rate</sub> = r<sub>rate</sub>

Equilibrium constant is Keq or Kc

 $K_{eq} (K_c) = [products]^x / [reactants]^y$ 

Percent Yield and Reaction Direction

Reactants can become products and products can become reactants % yield = (Actual / theoretical) x 100% No reaction (NR) < 1%Reactants favored >1% but < 50% Products favored >50% but < 99% To Completion >99% Chemical equation Need to know states Type of reaction Balance Givens Convert to moles Find molar ratio of solids Moles of product solid % yield = 4.84g / 5.90g x 100% % yield = 82.033898305%

# ∴ reaction is product favored Equilibrium Law (Keq)

#### K<sub>eg</sub> = [products]<sup>#mol</sup>/[reactants]<sup>#mol</sup>

- [] = concentration mol/L Keg has no units
- Keg and Kc are exchangeable
- Keq is temperature dependent
- Homogeneous equilibria: products and
- reactants are same phase
- All gases

Heterogeneous equilibria: products and reactants are different phase

 $\text{Liquid} \rightarrow \text{gas}$ 

Liquid (*I*): volume does not change, incompressible, constant is concentration Solids (s): incompressible, constant concentration

Gases (g): compressible, take shape and volume of container, concentration changes No liquids in Keq formula because [liquid is constant]

lons in solutions: aqueous solutions separate into ions, cancel out spectator ions K >>> 1, (K>=10<sup>3</sup>) forward reaction is preferred, equilibrium is to the right, more product forming Keq >10<sup>10</sup> reaction is complete K <<< 1 (K<10<sup>-3</sup>) reverse reaction is preferred, equilibrium is to the left, more reactant forming Keq >10<sup>-10</sup> no reaction happening K close to 1, reactant and products at equilibrium Keq is equilibrium concentration of chemicals with conditions Strategy to find  $k_{eq}$ : If question gives concentration at equilibrium and the equilibrium constant then solve for the missing concentration

Initial Change Equilibrium Table if question starts with initially or similar

- 1. Setup ICE table
- 2. Use E row in  $K_{eq}$  equation
- 3. Solve for unknown variables

Example Approximation rule question:  $K_{eq} = 4.5 \times 10^{-5}$ 

	CO <sub>(g)</sub>	$Br_{2(g)}$	COBr <sub>2(g)</sub>
Ι	2.20 mol/L	3.70 mol/L	0
С	-X	-X	+χ
E	2.20 -x	3.70 -x	x

3.70 / 6.7x10-5 = 55223.8806  $\therefore$  Yes it is more than 1000x difference, approximation

K<sub>eq</sub> = [Products] / [Reactants]

$$\begin{split} & \mathsf{K}_{eq} = [\text{COBr}_{2(g)}]^1 / [\text{CO}_{(g)}]^1 [\text{Br}_{2(g)}]^1 \\ & 6.7 \times 10^{-5} = [x]^1 / [2.20 - x]^1 [3.70 - x]^1 \\ & 6.7 \times 10^{-5} = x / (2.20)(3.70) \\ & 6.7 \times 10^{-5} = x / 8.14 \\ & (6.7 \times 10^{-5})(8.14) = x \\ & x = 5.45 \times 10^{-4} \text{ mol/L} \\ & [\text{COBr}_{2(g)}] = x \\ & [\text{COBr}_{2(g)}] = 5.45 \times 10^{-4} \text{ mol/L} \\ & [\text{Br}_{2(g)}] = 3.70 - x \\ & [\text{Br}_{2(g)}] = 3.70 - 5.45 \times 10^{-4} \end{split}$$

$$\begin{split} [Br_{2(g)}] &= 3.699455 \text{ mol/L} \\ [Br_{2(g)}] &= 3.70 \text{ mol/L} \\ [CO_{(g)}] &= 2.20 - x \\ [CO_{(g)}] &= 2.20 - 5.45 \times 10^{-4} \\ [CO_{(g)}] &= 2.199455 \text{ mol/L} \\ [CO_{(g)}] &= 2.20 \text{ mol/L} \end{split}$$

### **Reaction Quotient (Q)**

Find where the equilibrium of reaction is Use rate law to determine Q

To find location of the equilibrium, compare Q to  $K_{\mbox{\scriptsize eq}}$ 

If Q < K, reaction will move forward to get to equilibrium

If Q > K, reaction will reverse to get to equilibrium

If Q = K (within 0.1) the reaction is at equilibrium

Q equation is the same as  $K_{eq}$  but with the current concentration of all the reactants and products.

Example:

 $\begin{array}{l} \mathsf{K}_{\mathsf{eq}} = 4.0 \ \text{x10}^{-4} \\ [\mathsf{Br}_{2(g)}] = 3.70 \ \text{mol/L} \\ [\mathsf{CO}_{(g)}] = 2.20 \ \text{mol/L} \\ [\mathsf{COBr}_{2(g)}] = 5.45 \text{x10}^{-4} \ \text{mol/L} \end{array}$ 

 $Q = [COBr_{2(g)}]^1 / [CO_{(g)}]^1 [Br_{2(g)}]^1$ 

$$Q = [5.45 \times 10^{-4}] / [2.20][3.70]$$

Q =  $6.6953317 \times 10^{-5} < K_{eq} = 4.0 \times 10^{-4}$ 

 $\therefore$  rxn will proceed to get to equilibrium

# Le Châtelier's Principle

A chemical system at equilibrium opposes change when it is disturbed

<u>Concentration, moles, energy changes:</u> Increase in concentration of reactants will make the equilibrium shift to the right resulting in more products

Increase in concentration of products will make the equilibrium shift to the left resulting in more products

Decrease in energy of system will make the equilibrium shift to the left if endothermic and right if exothermic

Increase in energy of the system will make the equilibrium shift to the right if endothermic and left if exothermic <u>Volume and Pressure changes:</u> Boyle's law: P is inversely proportional to V P↑ V↓ means equilibrium will shift to the side with least total moles P↓ V↑ means equilibrium will shift to the side with most total moles <u>Catalyst:</u> No effect on concentration

Inert Gases: No effect on concentration Example Graph:



t1:The concentration of nitrogen is increased

t<sub>2</sub>: The pressure on the system is increased

 $t_3$ : The temperature is increased

# Solubility Product Constant (Ksp)

Molar solubility: the # of moles of solute that dissolves in 1L of solvent at a certain temp. Soluble compounds: completely dissociates into ions; no equilibrium

Insoluble compounds: only a tiny amount dissociates into ions; equilibrium

Solubility Product Constant (K<sub>sp</sub>): product of molar solubility and more solubility higher k<sub>so</sub>

General format  $K_{sp}$ : Solid (s) Aqueous ions (aq)

K<sub>sp</sub> = [A<sub>(aq)</sub>][B<sub>(aq)</sub>] / <del>[G<sub>(s)</sub>]</del> NO (solid)!! K<sub>sp</sub> is a measure of the solubility of a chemical

If  $\frac{K_{sp} \ll 0}{K_{sp} \gg 0}$  then low solubility; "insoluble" If  $\frac{K_{sp} \gg 0}{K_{sp} \approx 0}$  then high solubility; "soluble" Solve the same as  $K_{eq}$  problems.

 $[I] = 4.3x10^{-5} \text{ mol/L } [Ag] = 7.4x10^{-6} \text{ mol/L}$ K<sub>sp</sub> = [A][B]

 $K_{sp} = [4.3x10^{-5}][7.4x10^{-6}]$ 

 $K_{sp} = 3.182 \times 10^{-10}$ Predicting if a precipitate will form: Use ksp and Q

lf Q = K<sub>sp</sub>:

- At equilibrium
- No precipitate
- saturated solution

#### If $Q > K_{sp}$ :

- Right of equilibrium
- Precipitate
- Super saturated
- Many ions

# lf Q < K<sub>sp</sub>:

- Left of equilibrium
- No precipitate
- Not saturated
- Not enough ions
- K<sub>sp</sub> and Q example:

[I] =  $6.3 \times 10^{-5} \text{ mol/L} [Ag] = 8.4 \times 10^{-6} \text{ mol/L}$   $K_{sp} = 3.182 \times 10^{-10}$  Q = [A][B]  $Q = [6.3 \times 10^{-5}][8.4 \times 10^{-6}]$   $Q = 5.292 \times 10^{-10}$  $Q > K_{sp} \therefore$  a precipitate will form

# pH and pOH

<u>Acid:</u> chemical that releases hydrogen ion or hydronium ion when dissolved in water <u>Base:</u> any chemical that releases hydroxide ions (OH<sup>-</sup>) when dissolved in water Bronsted-Lowery:

<u>Brönsted-Lowry Acid</u>: chemical that <u>releases</u> a hydrogen ion  $(H^+_{(aq)})$  or hydronium ion  $(H_3O^+_{(aq)})$  when mixed with water

 $HF_{(aq)} + H_2O_{(aq)} \rightleftharpoons F_{(aq)}^+ H_3O_{(aq)}^+$ Acid Base Conj. base Conj. Acid Brönsted-Lowry Base: chemical that accepts a hydrogen ion (H<sup>+</sup><sub>(aq)</sub>) when mixed with water

 $CN_{(aq)}^{-} + H_2O_{(aq)} \rightleftharpoons HCN_{(aq)} + OH_{(aq)}^{-}$ Base Acid Conj. Acid Conj. base Conjugate acid/base pair: 2 molecules/ions that transfer [H<sup>+</sup>] in an acid/base reaction <u>DH:</u> measure of hydrogen ion concentration Examples: pH of HCl when [HCl] =  $3.45 \times 10^{-3} \text{ mol/L}$ pH =  $-\log[H^{+}_{(aq)}]$ pH =  $-\log[3.45 \times 10^{-3}]$ pH = 2.45Find [H<sup>+</sup>] of solution when pH = 4.54[H<sup>+</sup><sub>(aq)</sub>] =  $10^{-pH}$ [H<sup>+</sup><sub>(aq)</sub>] =  $10^{-4.54}$ [H<sup>+</sup><sub>(aq)</sub>] =  $2.88 \times 10^{-5}$  **pOH:** measure of hydroxide ion concentration pH of Ca(OH)<sub>2</sub> when [Ca(OH)<sub>2</sub>] =  $6.25 \times 10^{-2}$ mol/L

# pOH = -log[OH<sup>-</sup><sub>(aq)</sub>]

 $[H^{+}] = -\log[6.25 \times 10^{-2}]$   $[H^{+}] = 1.20$   $[H^{+}] = 1.20 \times \frac{1}{2}$   $[H^{+}] = 0.60$ What is the pH of a solution, pOH of 4.5? pH + pOH = 14

pH + 4.5 = 14pH = 9.5Find [OH<sup>-</sup>] of solution when pOH = 2.63[OH<sup>-</sup><sub>(an)</sub>] =  $10^{-pOH}$ 

#### $[OH_{(aq)}] = 10^{-2.63}$ $[OH_{(aq)}] = 10^{-2.63}$ $[OH_{(aq)}] = 2.34 \times 10^{-3}$

Sources: Cis/trans images: made in Molview Energy level diagram: <u>https://knowitinfo.com/what-is-energy-leveldiagram/</u> Vsepr summary chart: <u>https://www.pinterest.ca/pin/434175220306</u>

#### <u>021444/</u>

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