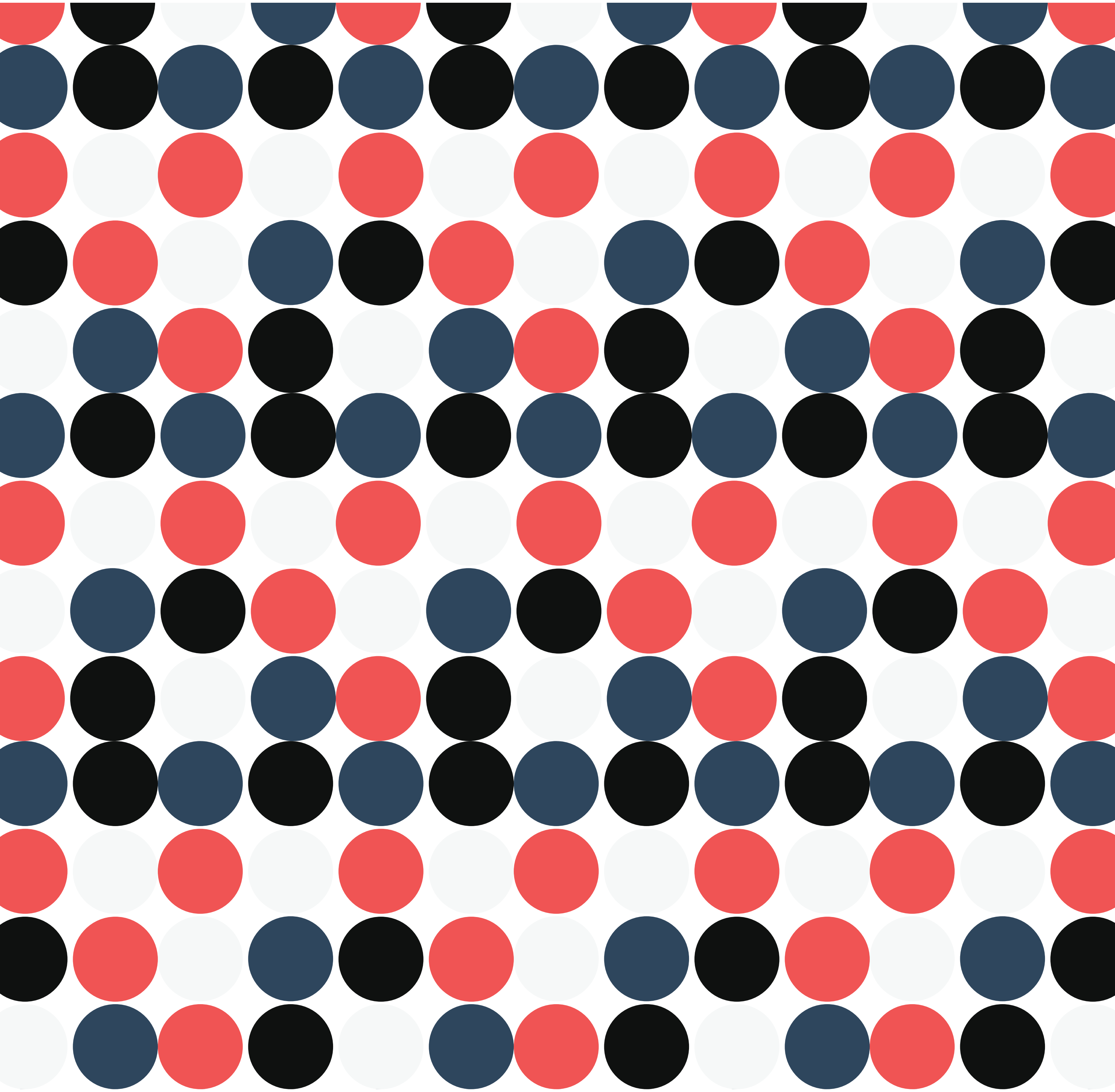

ELEMENTARY CHEMISTRY

An Infographic Guide

Patrick S. Firsan

Preface

Elementary Chemistry: An Infographic Guide was created to help eager students supplement their chemistry knowledge with key and concise information on chemistry topics ranging from introductory high school chemistry to introductory college chemistry. Color visuals and diagrams accompany each section to provide a more captivating and clearer depiction of the given chemistry topics. By making this project open access, I hope to reach students who may not have easy access to this information.

I would like to acknowledge and thank all the teachers who have inspired me so far and encouraged me to follow my curiosity both in and outside the classroom.

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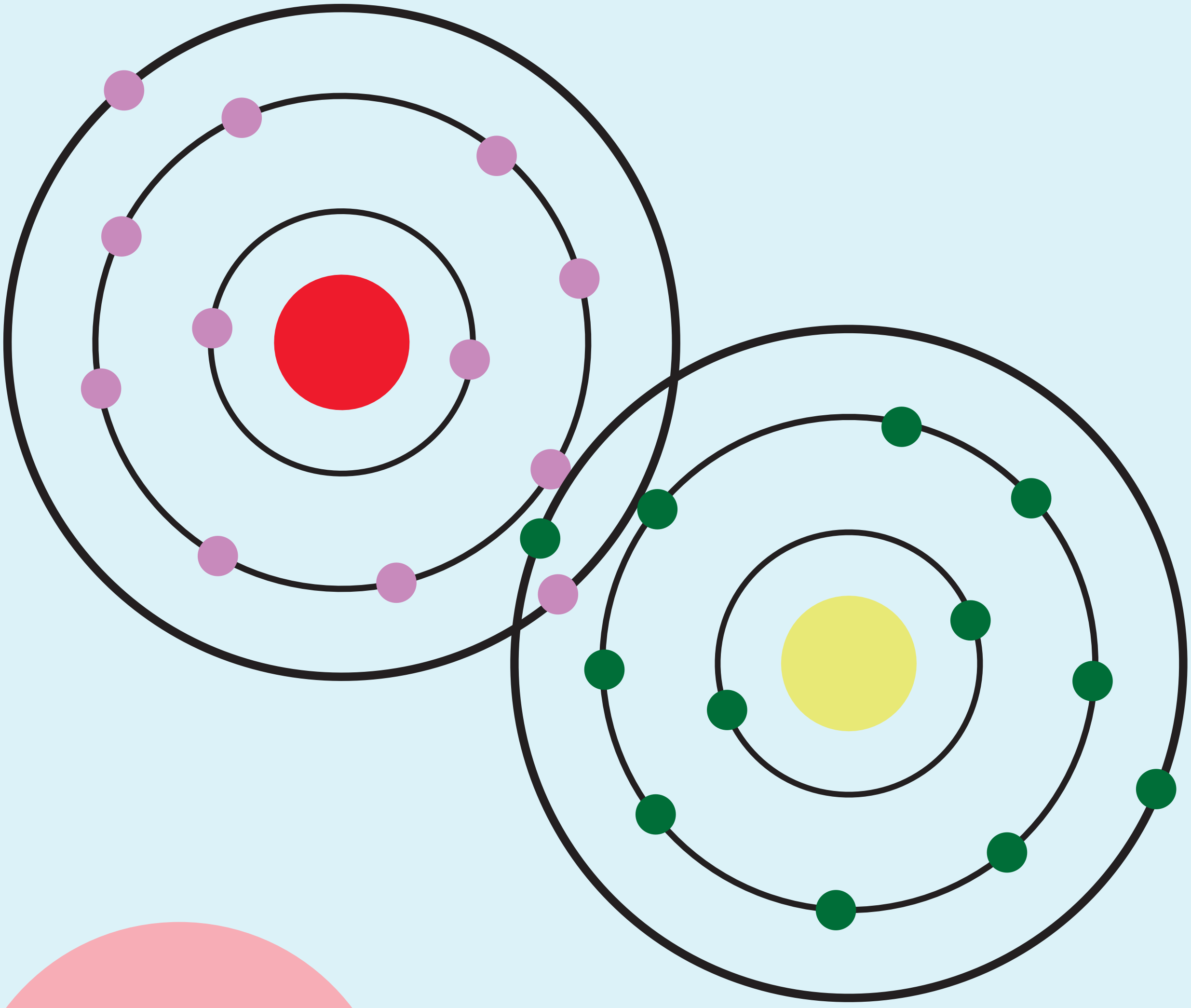
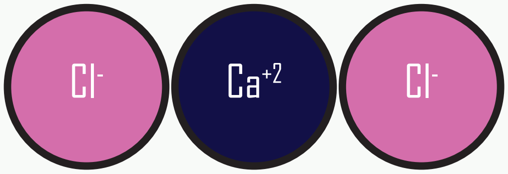


INTRODUCTORY CHEMISTRY

NAMING SYSTEMS

NAMING IONIC COMPOUNDS



It is understood that "calcium chloride" is to mean $CaCl_2$

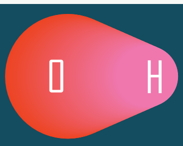
-Naming ionic compounds is rather elementary:

-Name the element on the leftmost side of the periodic table

-Name the other element; add an "-ide" suffix to it

*For the naming of ionic compounds, it is not important to name the number of elements (as in covalent compounds) because that number can often be understood from the name itself

NAMING COVALENT COMPOUNDS



-To begin, the name of the first nonmetal in the molecule (indicated by which element is farthest to the left in the periodic table) will be the first term in the name of the compound.

-For the second nonmetal, take the name and add an "-ide" suffix to it

-Add to both prefixes to indicate the number of each respective element in the compound.

-However, if the first nonmetal has "mono" as a prefix, "mono" is omitted because it is understood

-These rules are easier to see with some examples below

SiO_2 - Silicon Dioxide

CS_2- Carbon Disulfide

DIHYDROGEN MONOXIDE

(or by its more ubiquitous moniker, water)

Mono - one
Di - two
Tri - three
Tetra - four
Penta - five
Hexa - six
Hepta - seven
Octa - eight
Nona - nine
Deca - ten

MOLE CONVERSIONS

-Mole is an extremely important unit of measurement in chemistry

-A "mole" of something can be thought of like a "dozen"

-As a "dozen" represents 12 of something, a "mole" represents $6.02*10^{23}$ of something, in this case, particles

-Moles are important because they allow chemists to do comparisons between elements; an example of this is given below

Assume that you have 10.0g of two ionic compounds, lithium fluoride and silver chloride, and dissolve both samples in two beakers with an unspecified amount of water. You want to calculate the number of moles to see in which beaker there are more particles. To do so, you use the molar masses to find:

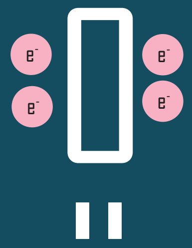
$$10.0\text{g} \times \frac{1\text{ mole}}{25.94\text{g}} = 0.386\text{ mol LiF}$$

$$10.0\text{g} \times \frac{1\text{ mole}}{143.32\text{g}} = 0.0698\text{ mol AgCl}$$

LEWIS STRUCTURES

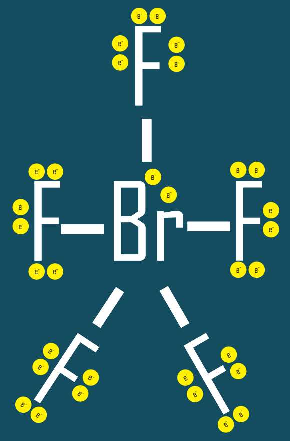
OCTET RULE (OR RULE OF EIGHT)

-The octet rule helps one draw Lewis structures
-It states that around each atom in a covalent molecule, there must be eight electrons around in its valence shell
-A covalent bond occurs when two atoms share two electrons; thus each bond represents two electrons



Exceptions to the Octet Rule

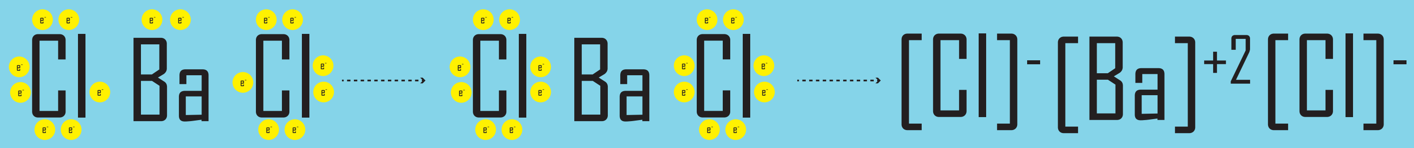
-While the Octet Rule is a general rule of thumb, not all elements follow it
-Boron and beryllium do not follow it. Beryllium only allows for four electrons around it while boron only allows six electrons
-Elements in the 3rd period of the periodic table and below may follow the octet rule, or they may have more than eight electrons around their valence shell in what is called an "expanded octet" (see the Lewis Structure of BrF$_5$ to the right)



DRAWING IONIC STRUCTURES

-The representation of ionic compounds is slightly different from the way covalent compounds are drawn

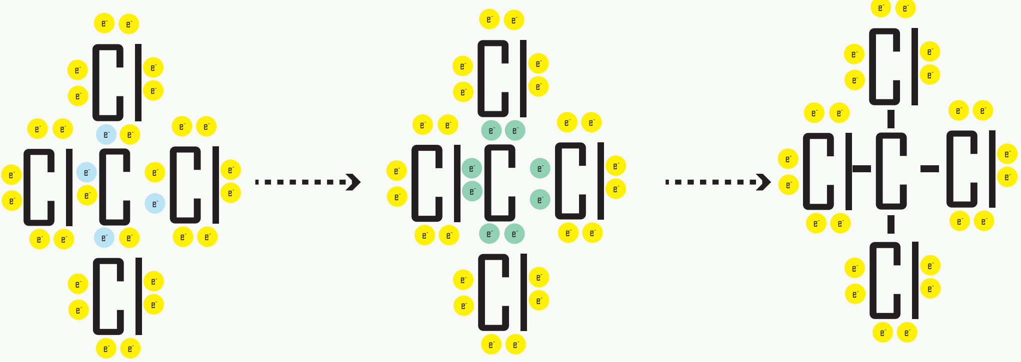
-The Lewis structure needs to show transfer of electrons and the charge on each ion
An example of this representation of this is shown below:



Showing the valence electrons

LEWIS STRUCTURES

HOW TO DRAW LEWIS STRUCTURES

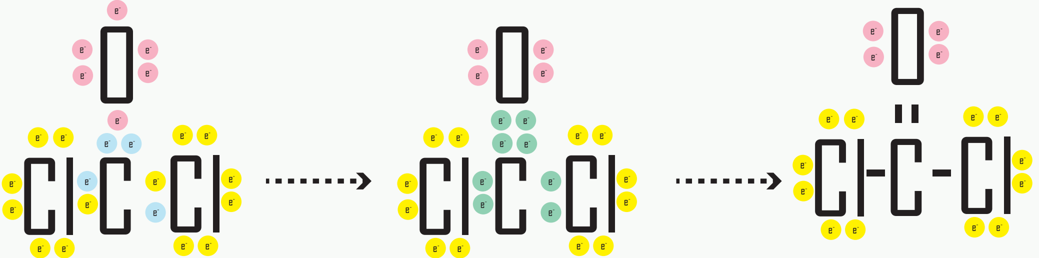


The blue dots represent carbon's valence electrons

The green dots represent the "shared" electrons

The shared electrons can then be represented by a solid line denoting a covalent bond

CARBON TETRACHLORIDE



The blue dots represent carbon's valence electrons
The pink dots represent oxygen's valence electrons

The green dots represent the "shared" electrons

The shared electrons can then be represented by a covalent bond

CARBONYL DICHLORIDE

1) Find the number of valence electrons in each atom of the molecule and add them up

In the case of carbon tetrachloride, each of the chlorines has 7 valence electrons and carbon has 4, meaning that, in total, there are 32 valence electrons

2) Begin Drawing

Write out the atoms as well as the number of valence electrons that each one has. In the case of carbonyl dichloride, six electrons have been drawn around the oxygen for its six valence electrons. Valence electrons are first put around each side of the atom and then paired

Tip: Try starting to draw out your structure by having the atom with the smallest number of valence electrons be the center atom. While this may not always be the case, the atom with the smallest number of valence electrons will need to have the most bonds to achieve the octet rule, thereby increasing the probability that it is the center atom

3) Make Connections

Connections need to be made to satisfy the octet rule. In the case of carbonyl dichloride. It can be seen that when originally drawn the octets of the chlorines are fulfilled with a single connection between each of them and the carbon. However, carbon still only has six electrons around it; so does oxygen. To resolve this, a double connection should be made between the carbon and oxygen.

4) Check

Count the number of electrons around each atom again. If there was only a single bond between the carbon and the oxygen, not only would the octet rule still not be fulfilled, but there would also be a single unpaired electron, which would still be incorrect. From this we see that there is a double bond between the carbon and oxygen

5) Recheck

Recounting ensures that all electrons have been used and paired and that the octet rule is satisfied for each atom in the Lewis structural formula

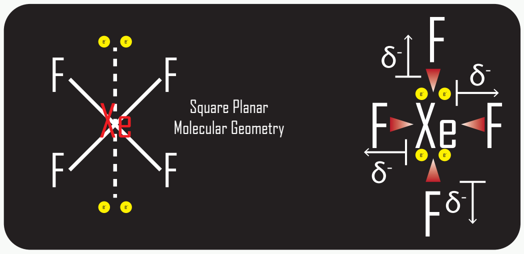
INTERMOLECULAR FORCES

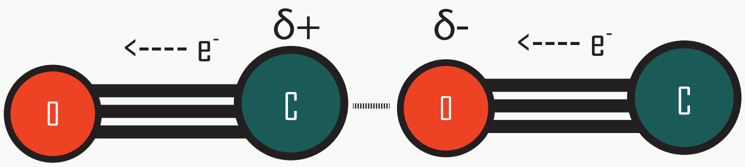
DIPOLE-DIPOLE FORCES

-Dipole-dipole forces are a type of intermolecular attraction created by the electronegativity difference between two covalently bonded atoms of a given compound

-This creates partial charges that allow for attraction

-It is important to note that while individual bonds may be polar, geometries may make the molecule as a whole nonpolar (as seen with XeF$_4$)





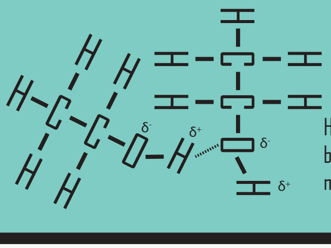
HYDROGEN BONDING

-Hydrogen bonding can be thought of as a special, much stronger type of dipole-dipole attraction

-A hydrogen bond occurs when a hydrogen is covalently bonded to a highly electronegative atom such as nitrogen, oxygen, or fluorine

-This in turn results in an extremely polar covalent bond due to the vast electronegativity differences between the hydrogen and either fluorine, nitrogen, or oxygen.

-This allows the molecule to form strong intermolecular attractions



Hydrogen bonding between two ethanol molecules

ION-ION ATTRACTIONS

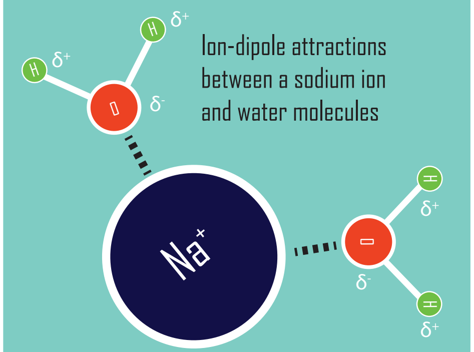
-Ion-ion attractions happen when the attraction is to each to such a degree that an electron gets kicked out of the atom with the lower electronegativity

-As a result, the charges on the atoms are permanent, making Ion-ion attractions the strongest type of intermolecular attractions

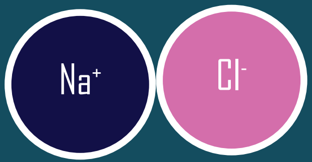
-The strength of an ion-ion attraction is related to the strength of the difference of the charges between the ions

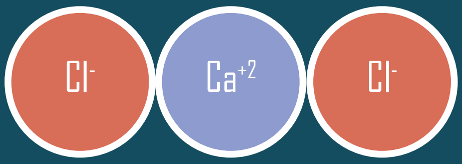
-The larger the difference the stronger the attraction

ION-DIPOLE ATTRACTIONS



Ion-dipole attractions between a sodium ion and water molecules





INTERMOLECULAR FORCES

LONDON DISPERSION FORCES

-The London Dispersion Force (or LDF) is the weakest force of attraction

-This is because LDF forces do not involve a permanent charge nor a partial charge, but a temporary partial charge

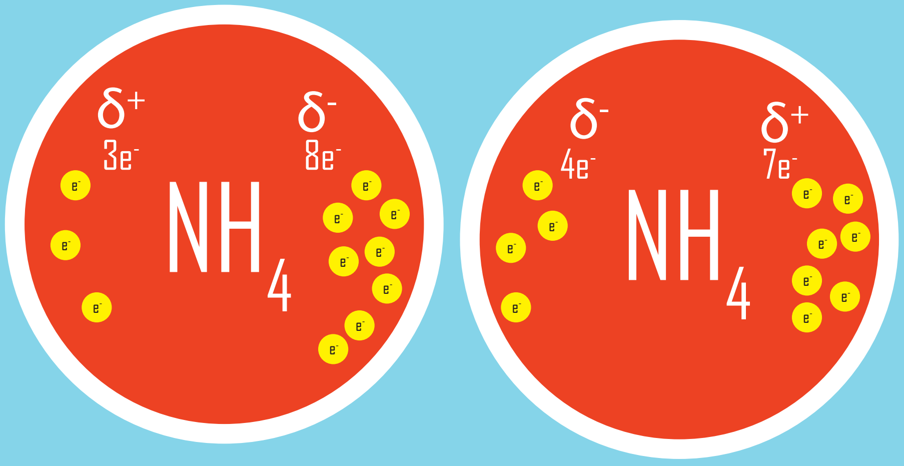
-How can a charge be temporary?

-When electrons swirl around in the molecule, inevitably due to the random whizzing of electrons in an atom, there will be a temporary imbalance of electrons creating a weak and TEMPORARY dipole moment in the molecule

-This dipole moment allows the molecule to become attracted to similarly nonpolar molecules

-An important thing to note is that, unlike with ionic and dipole forces where we focused on the valence shell of the molecule, LDF takes into consideration ALL the electrons in a molecule

-This means larger molecules will have stronger dispersion forces than smaller ones



A visualization of the London Dispersion Force

BALANCED EQUATIONS

HOW TO BALANCE A CHEMICAL EQUATION

___Fe + ___H_2SO_4 -> ___$Fe_2(SO_4)_3$ + ___H_2

_2_Fe + ___H_2SO_4 -> ___$Fe_2(SO_4)_3$ + ___H_2

_2_Fe + _3_H_2SO_4 -> ___$Fe_2(SO_4)_3$ + _3__H_2

$2Fe + 3H_2SO_4$ -> $Fe_2(SO_4)_3 + 3H_2$

1) Begin by balancing the easier term in the equation

First look at the iron and realize that while there are two irons in the products. There is only one in the reactants. Fix this by adding a 2 in front of the iron on the reactants side

2) Move on to the harder compounds

Now look at the sulfate. There are 3 of them in the products. To balance this add a 3 to the sulfuric acid in the reactants. As a result, there are now 6 hydrogens in the reactants but only 2 in the products. To balance the hydrogens, add a 3 in front of H_2 in the products.

3) Check

If all the terms of the equation are balanced, then the equation as a whole is balanced

CONVERTING WORD EQUATIONS INTO FORMULA EQUATIONS

Let us assume you were given the following reaction:
Calcium carbonate + hydrochloric acid -> carbon dioxide + calcium chloride + water
How would you go about writing the actual formula equation for the reaction? Some helpful hints for breaking it down are listed below
Calcium carbonate -> seeing the word "carbonate" makes one remember that carbonate is a polyatomic ion with a charge of -2 and that this is an ionic compound. As a result, you know that as calcium is in its ionic form it will have subsequently lost two electrons. As the charges balance, the formula is $Ca(CO_3)$
Hydrochloric acid -> This is an ionic compound and the lack of a numerical prefix (as well as the vast electronegativity difference between hydrogen and chlorine) gives that away. Chlorine's ionic charge is -1 and hydrogen's is +1, leading you to see the compound's formula is HCL
Carbon Dioxide -> the "di" prefix makes one remember that this compound is covalent. From here one can see that this compound will simply be single carbon with two oxygens, CO_2.
Calcium Chloride -> seeing the lack of a numerical prefix leads one to believe that this an ionic compound. Remembering from above you know that calcium in its ionic form will have a charge of +2 and chlorine will have a -1 charge. In order for these to balance to achieve a net charge of zero on the compound, there will have to be two chlorines. This leads one to conclude the compound's formula is $CaCl_2$
Water -> a ubiquitous moniker for H_2O
Combining everything from above results in the following formula equation: $CaCO_3 + HCl$ -> $CO_2 + CaCl_2 + H_2O$

FINDING THE LIMITING REACTANT IN A REACTION

Oftentimes when a chemical reaction occurs, while all of one reactant may get used up, there may still be some of the other reactant left over. The reactant that gets all used up is known as the “limiting reactant” (it limits how far the reaction can proceed), while the reactant that is leftover is known as the “excess reactant”. Instead of experimentally finding the limiting reactant, we can identify it by using dimensional analysis. Let us assume you were given the following reaction:

$$2Al + 3Cl_2 \rightarrow 2AlCl_3$$

You want to find the limiting reactant when 40 grams of aluminum and 50 grams of chlorine are used. To find this you do:

$$40.0\text{g} \times \frac{1 \text{ mole Al}}{26.98\text{g}} \times \frac{2 \text{ mole } AlCl_3}{2 \text{ mole Al}} = 1.48 \text{ mol } AlCl_3$$

$$50.0\text{g} \times \frac{1 \text{ mole } Cl_2}{70.91\text{g}} \times \frac{2 \text{ mole } AlCl_3}{3 \text{ mole } Cl_2} = \boxed{0.470 \text{ mol } AlCl_3}$$

As only 0.47 mol of $AlCl_3$ can be produced with 50 grams of chlorine, **chlorine would be considered the limiting reactan**t in this scenario

SOLUTIONS AND CONCENTRATIONS

CALCULATING MOLARITY AND MOLALITY

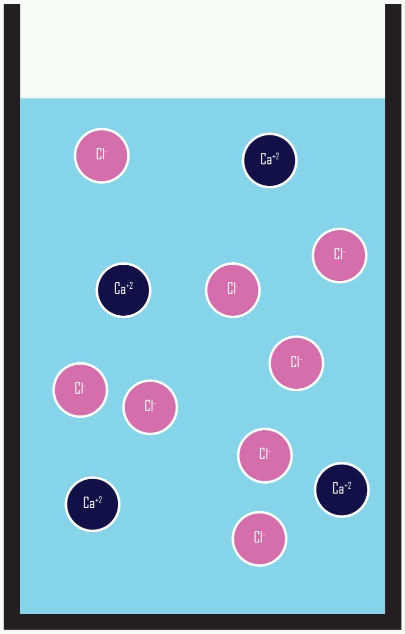
(UNITS OF CONCENTRATION)

-The formula for molarity is:

$$M = \frac{mol}{L}$$

-The formula for molality is:

$$m = \frac{mol}{kg}$$



Example

Assume you just put in 55.49 grams of calcium chloride in 2 liters of water. Using dimensional analysis, you find that you put in 0.5 moles of calcium chloride in the water. Thus, you find that the molarity is 0.25 mol/L. Then by using water's density of 1 kg/L, you find that 2 liters of water weigh 2 kg meaning the molality is 0.25 mol/kg

FINDING NET IONIC EQUATIONS

For our purposes, let us assume that you were given the following equation

$$AgNO_3(aq) + KCl(aq) \rightarrow AgCl(s) + KNO_3(aq)$$

1) Disassociate the soluble compounds in the equation

$$Ag^+ + (NO_3)^- + K^+ + Cl^- \rightarrow AgCl + K^+ + (NO_3)^-$$

2) Balance

$$Ag^+ + (\cancel{NO_3})^- + \cancel{K}^+ + Cl^- \rightarrow AgCl + \cancel{K}^+ + (\cancel{NO_3})^-$$

3) Remove Spectator Ions

$$Ag^+ + Cl^- \rightarrow AgCl$$

SPECTATOR IONS

-Spectator ions are ions that are present both at the beginning of a reaction and remain unaffected by the end of it

-As a result, when writing out reactions, they are unimportant (as nothing occurred to them, they were just merely "spectators" to the actual reaction) and are thus crossed out

SOLUTIONS AND CONCENTRATIONS

FINDING IF A COMPOUND IS SOLUBLE

(For example in water)

-The solubility of a molecule is directly related to its polarity
-In order for a compound to be soluble, its intermolecular forces need to be stronger than the solvent's
-For our purposes we will focus on water; water uses hydrogen bonding for its intermolecular forces
-For a compound to be soluble, water needs to disassociate from itself and re-associate with the compound to be dissolved (the solute)

-Ionic compounds are soluble in water

-Why? This is because (remember earlier) ionic compounds have permanent charges on the atoms that make them up. Permanent charges are very strong and this makes it favorable for them to separate the water molecules from each other

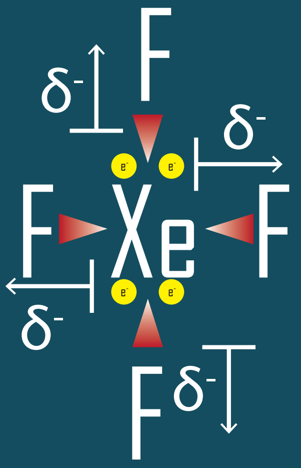
-Compounds that use dipole-dipole attractions are soluble in water

-Why? This is because while dipole-dipole attractions are slightly less strong than hydrogen bonding, the partial charges are still strong. This makes it attractive for water to disassociate and re associate to the compound and allows for the compound to dissolve

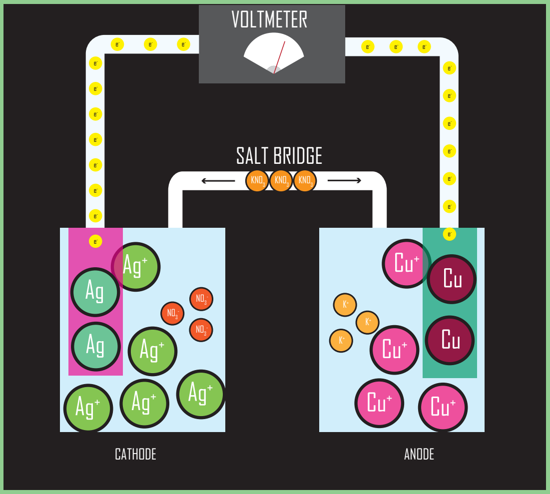
-Compounds that use London Dispersion forces as their intermolecular force of attraction are insoluble

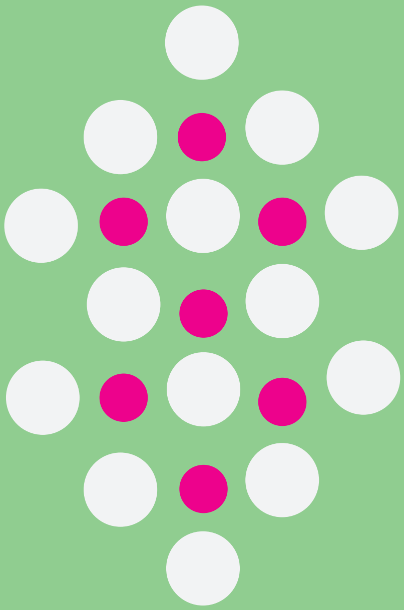
-Why? This is because LDF transposes a temporary charge. The strength of and the charge itself of the molecule will come and go depending on the electron distribution within the molecule. As a result, it is unfavorable for water to disassociate from itself and form attractions with these compounds. That makes these compounds insoluble in water

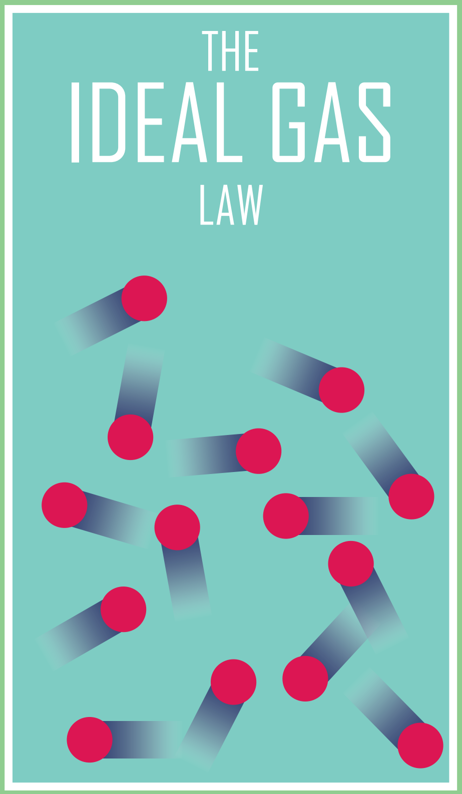
-A rule of thumb for predicting solubility is **"like dissolves like"**

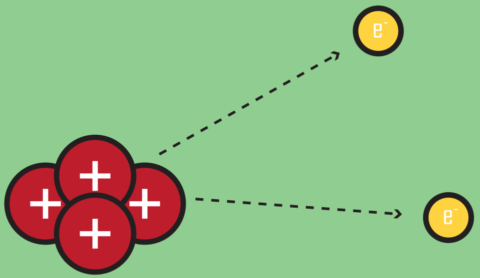


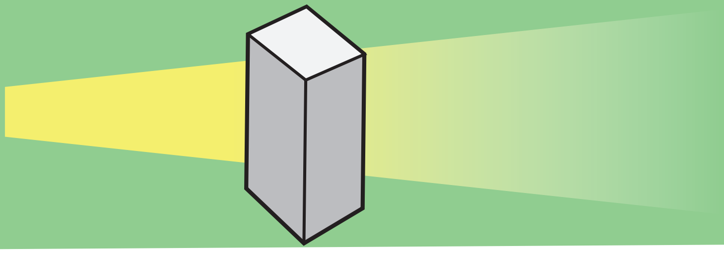
XeF_4 is a nonpolar molecule, and as a result, it is **NOT** soluble in water

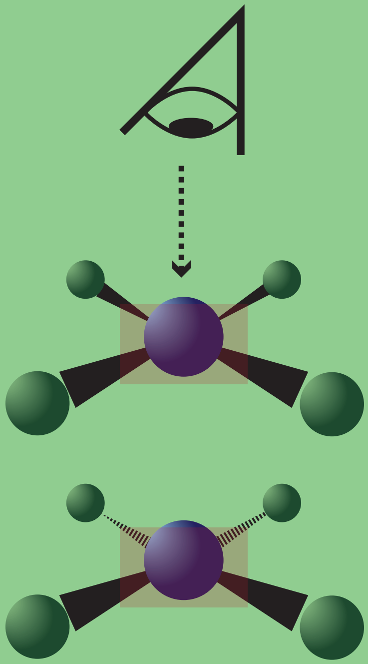




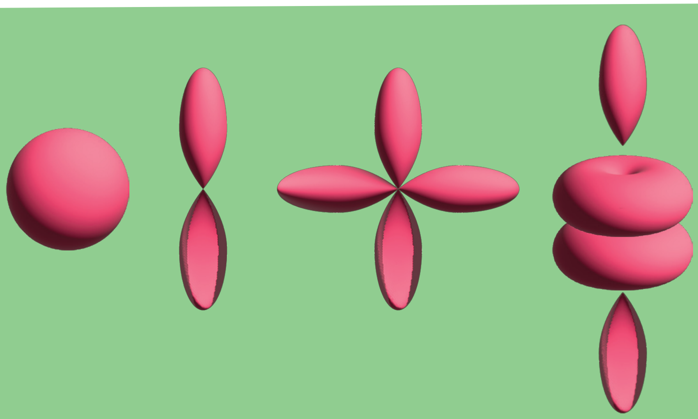


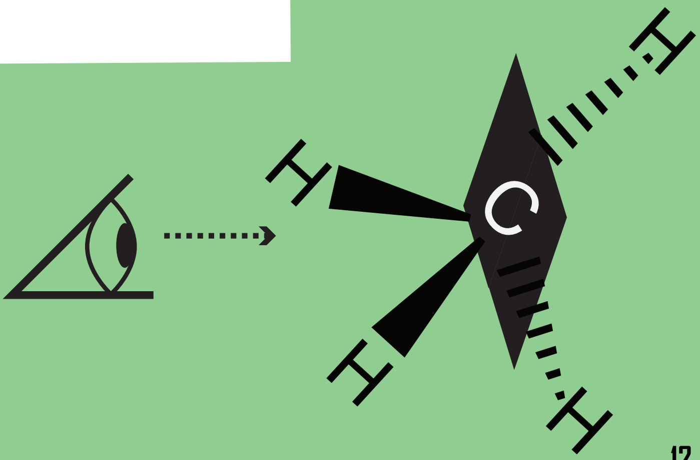






ADVANCED CHEMISTRY





LIGHT AND WAVES

WAVE-PARTICLE DUALITY AND EMR

-While you may not realize it, everything around us behaves as a particle or object and as a wave

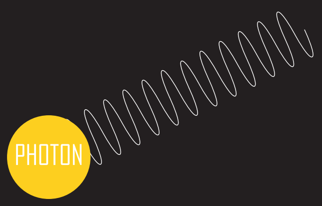
-While investigating the nature of light, Einstein hypothesized that light behaved in two ways: as a photon (a particle) and also as a wave

-The Electromagnetic Spectrum was created to describe the different types of wavelengths that exist (and accordingly, their respective frequencies)

-Different wavelengths have different applications and uses, many of which are commonly found in everyday life.

-Interestingly, visible light is on the electromagnetic spectrum and from it, we can see that specific wavelengths of visible light correspond to the different colors that we see

-This is especially important to take note of when doing colorimetry experiments



Light behaving as a wave and a particle: wave-particle duality

RELATIONSHIP BETWEEN ENERGY, SPEED OF LIGHT, FREQUENCY AND WAVELENGTH

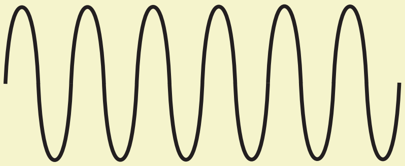
-There are two properties that are used to describe the different types of waves in the electromagnetic spectrum

-Frequency is the number of cycles (or "periods") over a certain time interval

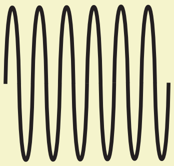
-Wavelength is the measure of the length of a single cycle or period

-It is important to note that frequency and wavelength are inversely related: a longer wavelength will have a smaller frequency and a shorter wavelength will have a larger frequency.

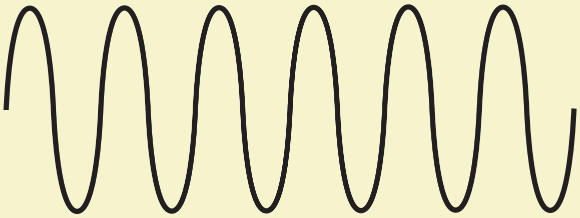
-This is illustrated by the figure above



Longer Wavelength
Smaller Frequency



Shorter Wavelength
Larger Frequency



Two equations come from this

$C = \lambda v$

-"C" is the constant for the speed of light
-"λ" represents the wavelength
-"v" stands for the frequency; its measured in 1/s or s^{-1}

$E = hv$

-"E" represents the amount of energy in joules for a single photon
-"h" represents Planck's constant: approximately $6.634 * 10^{-34}$
-"v"stands for the frequency; its measured in 1/s or s^{-1}

LIGHT AND WAVES

ELECTRONIC CONFIGURATION

-An atom's electronic configuration describes the arrangement of electrons around its nucleus

-Electrons are described to be in different orbitals--types of 3-dimensional geometries around the nucleus that describe high probabilities of where an electron will be at any given moment

-Orbitals are organized by energy levels as well as the different 3 dimensional spaces around the atom

There are 4 different types of orbital: s, p, d, and f

-s orbitals can hold two electrons
-p orbitals can hold six electrons
-d orbitals can hold ten electrons
-f orbitals can hold fourteen electrons

-To find the electronic configuration of an atom:

-Realize that by adding up the sum of the orbital numbers exponents should equal the atomic number of an element

-Realize that coefficients represent energy levels

-The orbitals of the first few elements fill up with this pattern

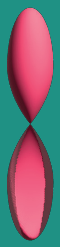
-$1s^2$
-$2s^2\ 2p^6$
-$3s^2\ 3p^6$
-$4s^2\ 3d^{10}\ 4p^6$

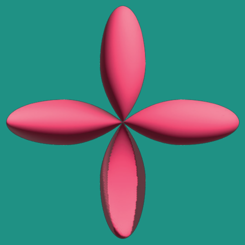
-As an example, the electronic configuration for nitrogen is $1s^2\ 2s^2\ 2p^3$. This makes sense as 2+2+3 = 7 which is nitrogen's atomic number

-To simplify electronic configurations, you can put the atomic symbol of the noble gas that came before the element you are trying to find the electronic configuration for. For example, the electronic configuration of Ti would be [Ar] $4s^2\ 3d^2$

-It is also important to note that while the 3d orbital is written after the 4s orbital, one considers the valence electrons to be those in 4s because it is in a higher energy level (4 v 3) than 3d


s-orbital


p-orbital


d-orbital


f-orbital

GASES

IDEAL GAS LAW (IGL)

The Ideal Gas Law helps solve for unknowns when some condition of a gas is known

The equation is broken down below

- -P stands for pressure; measured in atmospheres (atm)
- -V stands for volume; measured in liters (L)
- -n stands for the number of moles of the substance; measured in moles (mol)
- -R stands for a constant that is equal to .0821 (L*atm)/(mol*K)
- -T stands for temperature; measured in Kelvin (K)

-Standard Temperature and Pressure (STP) conditions are 1 atm and 0 °C

-To see how conditions change when a variable or property of a gas changes, you can use the following equation:

$$(P_1V_1)/(n_1R_1T_1) = (P_2V_2)/(n_2R_2T_2)$$

-One can ignore conditions that stay the same in both scenarios

-For example, if you want to see how the pressure is affected when the volume is halved. The volume was originally 4L and the pressure was 2 atm

-Putting $P_1V_1 = P_2V_2$ one finds that (2)(4) = $(P_2)(2)$; solving you find that P_2 is 4 atm

RELATION BETWEEN IDEAL GAS LAW VARIABLES AND BETWEEN IGL AND KINETIC ENERGY

As the ideal gas law is an equation, some relationships between variables can be identified. These are listed below:

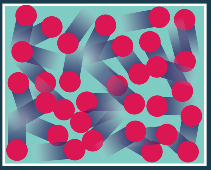
- -P and V are inversely related
- -T and n are inversely related
- -P and n are directly related
- -V and n are directly related
- -P and T are directly related
- -V and T are directly related

$$PV=nRT$$

-The ideal gas law and kinetic energy:

- -Temperature is a measure of the **average kinetic energy** in a system

DEVIATIONS FROM IDEAL GAS LAW



At high pressures, the molecules can no longer behave as a gas

-While the Ideal Gas Law is a very helpful tool, it cannot always be relied on since not every substance or situation is "ideal"

-Most notably, the ideal gas law is not accurate when molecules are polar

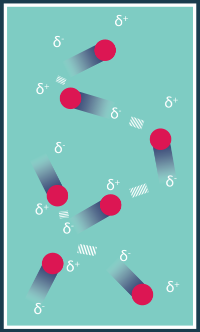
Why? Because when molecules are polar, they are able to attract each other better, which then messes up the dynamic of the gas particles

-This is shown in the figure to the right

-The ideal gas law is also not accurate when the pressure inside of a system is too great

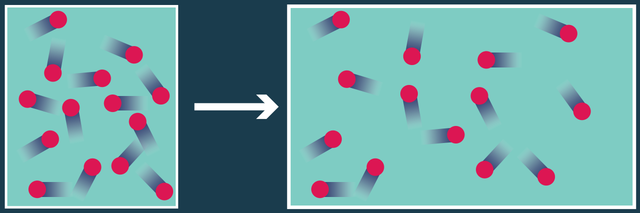
-Why? When the pressure becomes too high, the molecules no longer behave like a gas, but instead there is so little room to move around that the gas becomes liquid-like

-This is shown in the figure to the right

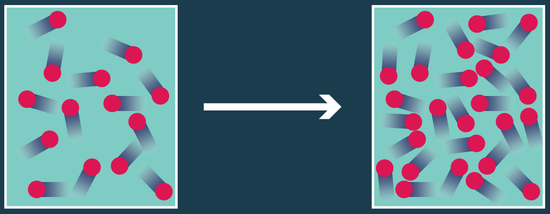


Molecule polarity interferes with gas behavior

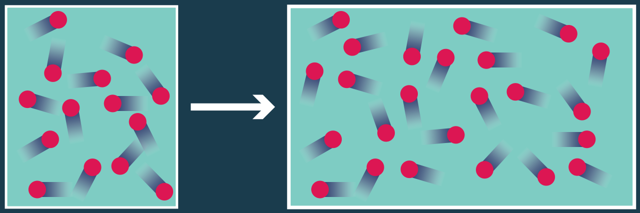
THE IDEAL GAS LAW



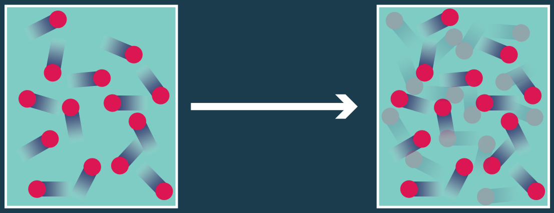
As volume increases, the number of collisions decreases, thereby decreasing the pressure in the system



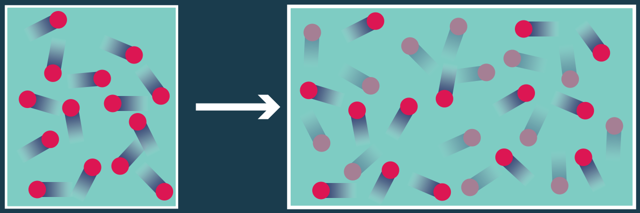
As the number of moles increases, the number of collisions will increase, thereby increasing the pressure in the system



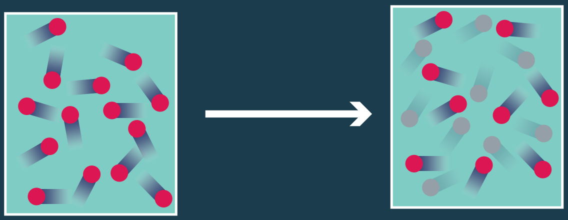
As volume increases, the number moles that the system can sustain increases



As the temperature increases, the average kinetic energy in the system increases, increasing the number of collisions, which is the pressure



As the temperature increases, in order to sustain a certain pressure, the volume has to increase



As the temperature increases, the average kinetic energy in the system increases, thereby decreasing the number of moles needed to attain a certain pressure

BONDING

RELATION BETWEEN CONDUCTIVITY, MELTING POINT, SOLUBILITY, AND INTERMOLECULAR FORCES

-If I asked you which metal will be a better conductor of electricity, how would you know?

-The molecular properties of melting point, solubility, and conductivity are all related to the **strength of intermolecular forces**

-Melting point refers to the temperature at which a compound changes its physical state of matter from being a solid to being a liquid

-**Conductivity** refers to the ability of a compound to **transfer electric current or temperature**

-**Solubility** refers to the **ability of a compound to dissolve** in a solvent (oftentimes water but can be various other liquids depending on the situation)

-In order for a substance to have a high melting point, it needs to have **strong intermolecular forces**

-Why? Stronger intermolecular forces are harder to break: this means more energy is required to turn the substance from a solid to a liquid

-In order for a substance to be soluble, one has to take into consideration the **solute's and the solvent's intermolecular forces**

-Why? Compounds do not generally disassociate and form weaker attractions. For example, if I put ethylene (C_2H_4) into water, a nonpolar compound that bonds using LDF, it will not dissolve in water because water molecules use hydrogen bonding to form their intermolecular forces of attraction which is much stronger than LDF.

-However, glucose ($C_6H_{12}O_6$) is able to dissolve in water because its OH groups make the molecule polar. In this scenario, the water molecules are willing to disassociate from each other and attract to the glucose, thereby dissolving the glucose

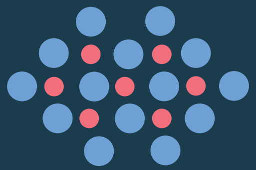
-In either scenario, the polar compounds do not want to disassociate from themselves and form weaker attractions with other molecules

-In order for a substance to be a good conductor of electricity, **its electrons need to be able to move around relatively freely**

-This is true with metallic bonding but also with dissolved (not solid) ionic compounds

-Why dissolved ionic compounds? When the substance is dissolved, its particles are able to move more freely as compared to when it is a solid and the permanent charge difference between compounds facilitates electron transfer

LATTICE ENERGY AND ELECTROLYTES



-Lattice energy describes the energy required to break apart an ionic solid

-Ionic compounds with a bigger difference between their positive and negative charges will require more energy to break apart

-$MgCl_2$ will require more energy to break apart than NaCl

-NaCl has a +1 and a -1 charge on the sodium and chloride, respectively

-$MgCl_2$ has a +2 and -1 charge on the magnesium and each chloride, respectively

-Why? This relates to nuclear charge -> bigger difference in charge means less electrons but the same number of protons

-Magnesium can pull on its electrons more and the resulting ionic compound will be smaller and more tightly held

-Electrolytes are solutions of dissolved ions

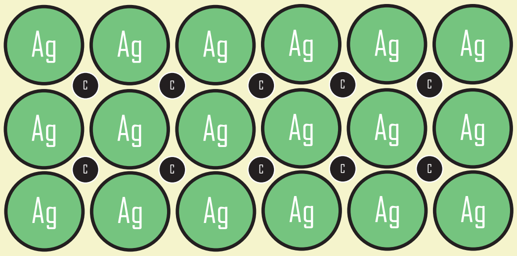
-Electrolytes are able to conduct electricity because the dissolved ions are able to move more freely in the solvent

BONDING

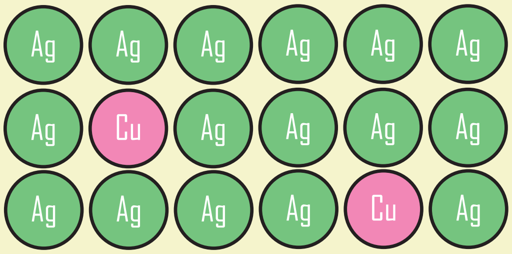
METALLIC BONDING & ALLOYS

-Metals (specifically transition metals) bond differently from other elements
-Transition metals bond by forming a lattice together; this is known as "metallic bonding"
-In this lattice, each of the atom's valence electrons "delocalize" or are no longer bound by the confines of the atom but instead move in the surroundings around it
-Delocalization is possible because of the large distance between the valence electrons and the nucleus
-This results in a "sea of electrons" to form around the atoms (this is depicted to the right)
-As the electrons are able to move around much more freely, this results in metals being very good conductors of electricity and heat

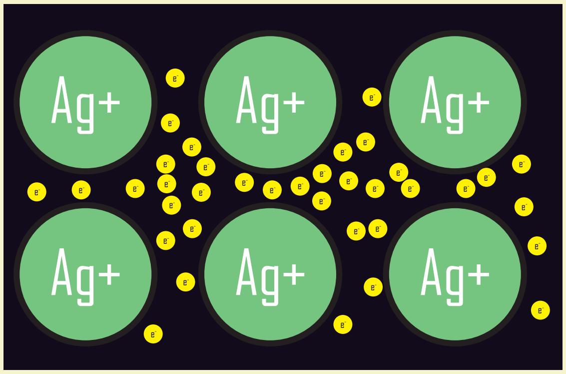
-Alloys are a composition of two or more different metal elements. There are two types of alloys:
-Interstitial alloys are when a different element is added in-between the gaps of the metal atoms of the first metal.
-Substitutional alloys are when the alloy's lattice is comprised of two different elements in varying proportions.



Interstitial Alloy



Substitutional Alloy



Metallic Bonding

CHARGE AND SPECTROSCOPY

EFFECTIVE NUCLEAR CHARGE AND SHIELDING

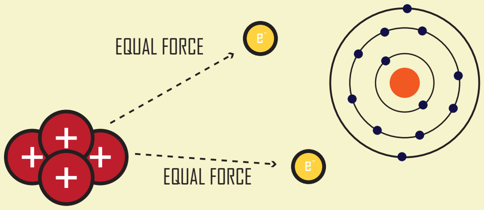
-The effective nuclear charge refers to the attractive force that the electrons in the various orbitals feel from the nucleus of an atom

-The strength of a nuclear charge is affected by the following

Distance: What energy level are the electrons in?

Protons: How many protons are in the nucleus?

Electrons: Electrons can cause repulsions and electron shielding of other electrons



A figure demonstrating Coulomb's Law

-It is important to note that a proton does not "split up" its force; that is when there are two electrons that are equidistant from the nucleus, they will both feel the same force from the protons in the nucleus. This is known as Coulomb's Law.

BEER'S LAW

$A = \varepsilon bC$

Beer's law is used during colorimetery measurements. It is:

$$A = \varepsilon bC$$

Breaking it down:

-"A" stands for the absorbance

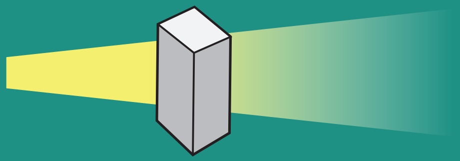
-"ε" stands for the molar absorptivity

-"b" stands for the length of the light path in the measuring cell

-"C" stands for the concentration of the substance

-In essence, it states that absorbance is related to the concentration of a substance--the more molecules there are, the more that can absorb the wavelength

-This concept is most clearly seen when one places different concentrations of a solution into multiple cuvettes and then tests them for absorbance by using an acceptable wavelength that can be absorbed by that substance



As light passes through the cuvette, it becomes absorbed by the molecules inside the cuvette

PES DATA AND SUCCESSIVE IONIZATION ENERGIES

-PES stands for "photoelectron spectroscopy"

-PES Graphs are usually depicted like the one shown on the right ---->

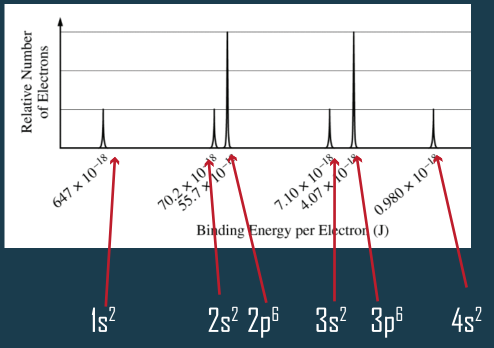
-PES Graphs show the amount of energy required to remove an electron in a specific orbital out of the atom

-Electrons in lower energy levels will require significantly more energy than the atom's other electrons to be kicked out of the atom due to their proximity to the nucleus

-Electrons in higher energy levels will require significantly less energy than the atom's other electrons to be kicked out of the atom due to their distance from the nucleus

-Thus, as a result, one can easily determine which electrons are being referred to in each peak of the graph by counting electrons, or by counting each peak as another orbital shell

-This is shown to the right

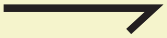


From AP® Central AP Chemistry 2019 Exam FRQ Question #5

REACTION MECHANISMS

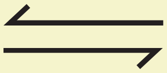
STRAIGHT ARROWS

A straight arrow represents the movement of an **electron pair**

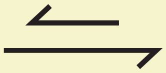


Half of a straight arrow represents the movement of a **single electron**

A straight arrow can also represent the reaction only moving in **one direction**



Represents a reaction that goes to an **equilibrium**



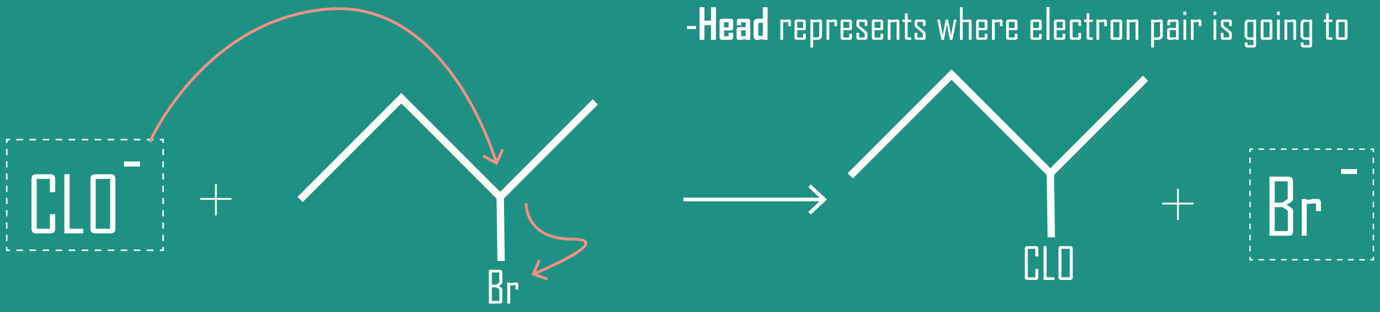
Represents a reaction that goes in both directions but the equilibrium favors one side

CURVED ARROWS

-Curved arrows help show how electrons are moving in a reaction

-**Tail** represents where electron pair is coming from

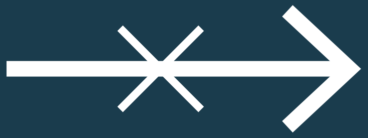
-**Head** represents where electron pair is going to

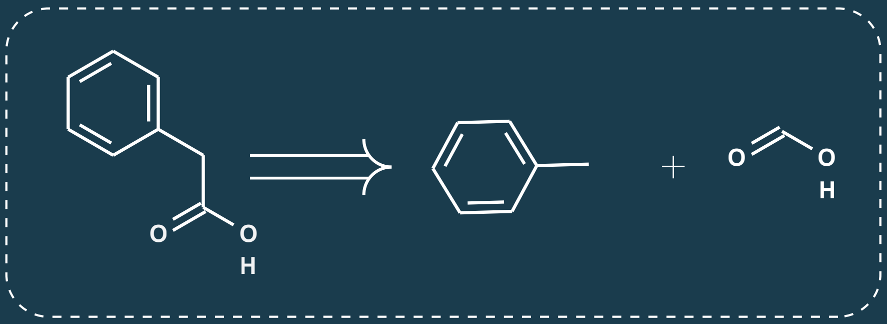


NO REACTION & RETROSYNTHESIS ARROWS

-Retrosynthetic arrows are meant to show how the compound came about; what it was made from

The no reaction arrow shows that the reaction will not occur

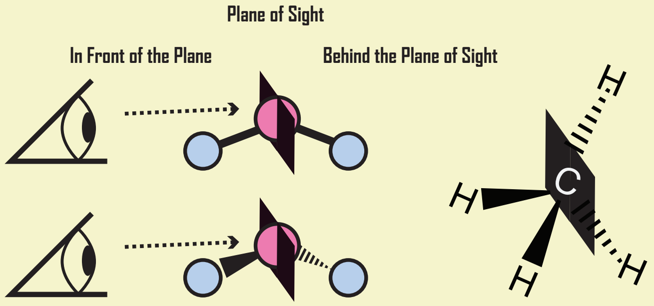


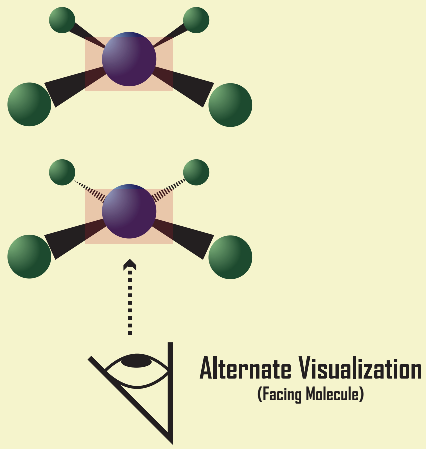


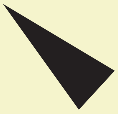
ADVANCED ATOMIC MODELS

DASHED AND SOLID WEDGES

Representing Orientations of Bonds in Space (3D)



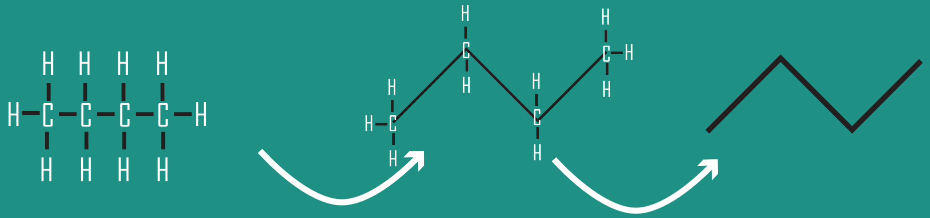




A solid wedge means that the bond is coming towards you

A dashed wedge means that the bond is going away from you

SKELETAL (BOND-LINE) STRUCTURE



-Once structures become larger and increasingly more and more complex a more simplified type of structure is needed to represent molecules

-Each "peak" or "valley" or "vertex" represents a carbon atom with the appropriate number of hydrogens bonded to it given its position in the structure. In this example it is either two or three (as shown above) depending on whether or not the carbon is in the middle or end of the structure

-This logic can also be applied to aromatic rings

-Thus, carbons and hydrogens are not drawn: they are just implicitly known

-Elements other than carbon and hydrogen have to be written in or shown in the structural formula

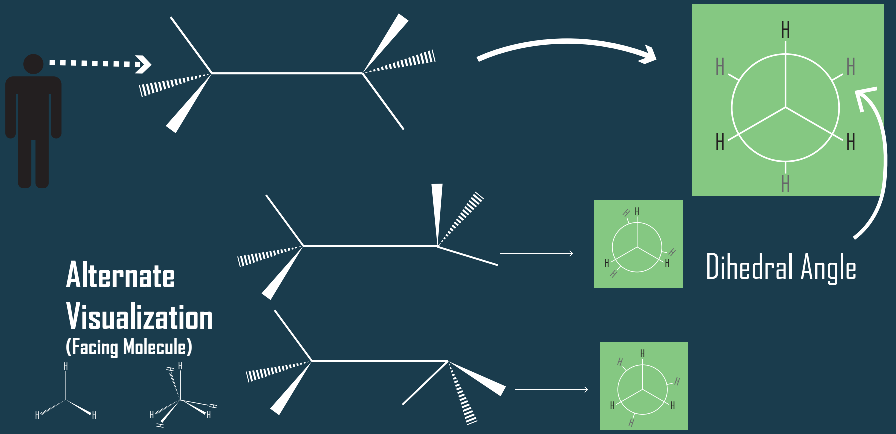
CONDENSED STRUCTURE

The condensed structure of the compound is a way to write out the structure by more clearly stating which atoms and groups bond to each other

For example, the condensed structure of the structure to the bottom and left (butane) is $CH_3(CH_2)(CH_2)CH_3$

NEWMAN PROJECTION

Newman Projections are used to represent different conformations of molecules



-Compounds can have multiple different "conformations" or orientations or rotations of bonded atoms in 3-dimensional space

-Newman Projections are used to show these differences

-Newman Projections are drawn as if one is facing the molecule and can see the front and back like a 2D snapshot of the molecule

-When structures are drawn like this, one can look at the angle formed between the front and back atoms

-These angles are called dihedral or torsional angles

-The dihedral angles are important because of the differences in potential energy between conformations

-**Staggered formation**: the conformation resulting in lowest potential energy of the molecule

-**Eclipsed formation**: the conformation resulting in the highest potential energy

BONDS

RESONANCE STRUCTURES & FORMAL CHARGES

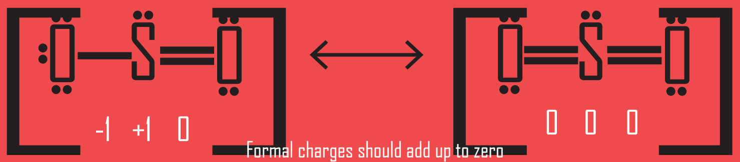
-A resonance structure is when a molecule has bond lengths that do not fit the length of a single bond, double bond, or even a triple bond. Instead, the bond lengths are between these lengths (i.e. between the length of a single or double bond).
-Thus, in order to account for this, resonance structures were created

-**Formal Charges** help one see which resonance structure may be the most "accurate"
-In order to calculate the formal charges, one must first count the number of electron pairs on an atom. Then one should count the number of electrons from bonds and divide them by two.
-Then, one should subtract these numbers from the number of valence electrons each atom would normally have. The more stable structure will be the one with:

1) The **least formal charges**
2) The **least separation** between formal charges
3) The **negative charge** on the **more electronegative** atom

-An example is shown below and from it you can see that the structure on the is the more right is the stable one for sulfur dioxide
-But remember that the truly correct structure is neither but rather a combination of the two

RESONANCE STRUCTURES

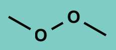


Formal charges should add up to zero

ISOMERS

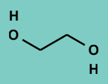
Isomers are compounds that share the exact **same chemical formula but differ in structure**.
There are two classes of isomers: constitutional isomers and stereoisomers. Constitutional isomers have the same molecular formula but different bonding of elements in the molecule. Stereoisomers have the same molecular formula but have a different 3-dimensional configuration of them.

We will go into greater detail on that later on. For now, just understand that they are molecules with the same formula but have different configurations of their shared composing elements. An example of two constitutional isomers is given below:



Dimethyl Peroxide

$C_2H_6O_2$

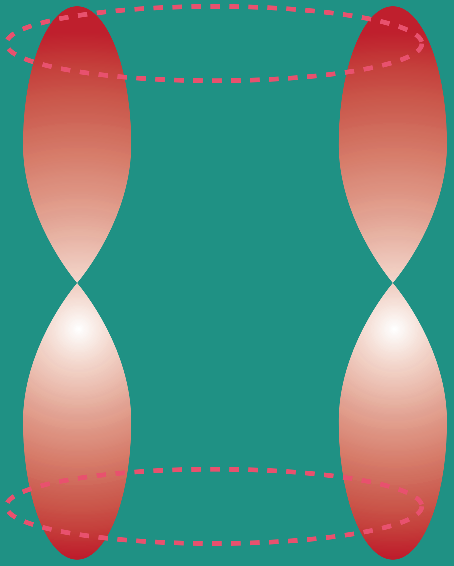


Ethylene Glycol

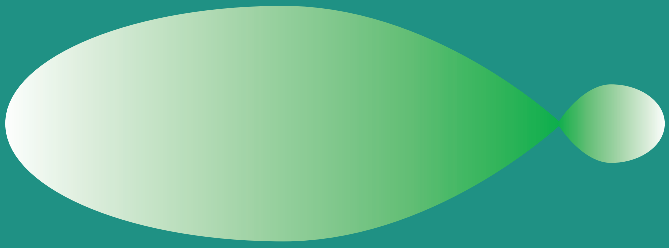
HYBRIDIZATION

-Science has multiple theories of bonding
-One of these, is known as "hybridization"
-Hybridization was created to explain bond lengths
    -P orbitals have a higher energy than s and should thus have shorter bond lengths
    -In actuality this is not the case; for example for methane (CH_4), all the bond lengths are the same
    -To explain this phenomenon, the concept of hybridization was created
-To put it very simply, during hybridization, the valence shells of two atoms will essentially merge together
-The hybridization in the following scenarios are listed below:
    -1 connection to another atom or lone pair: s
    -2 connections to another atom or lone pair: sp
    -3 connections to another atom or lone pair: sp^2
    -4 connections to another atom or lone pair: sp^3
    -5 connections to another atom or lone pair: sp^3d
    -6 connections to another atom or lone pair: sp^3d^2

Pi bonds



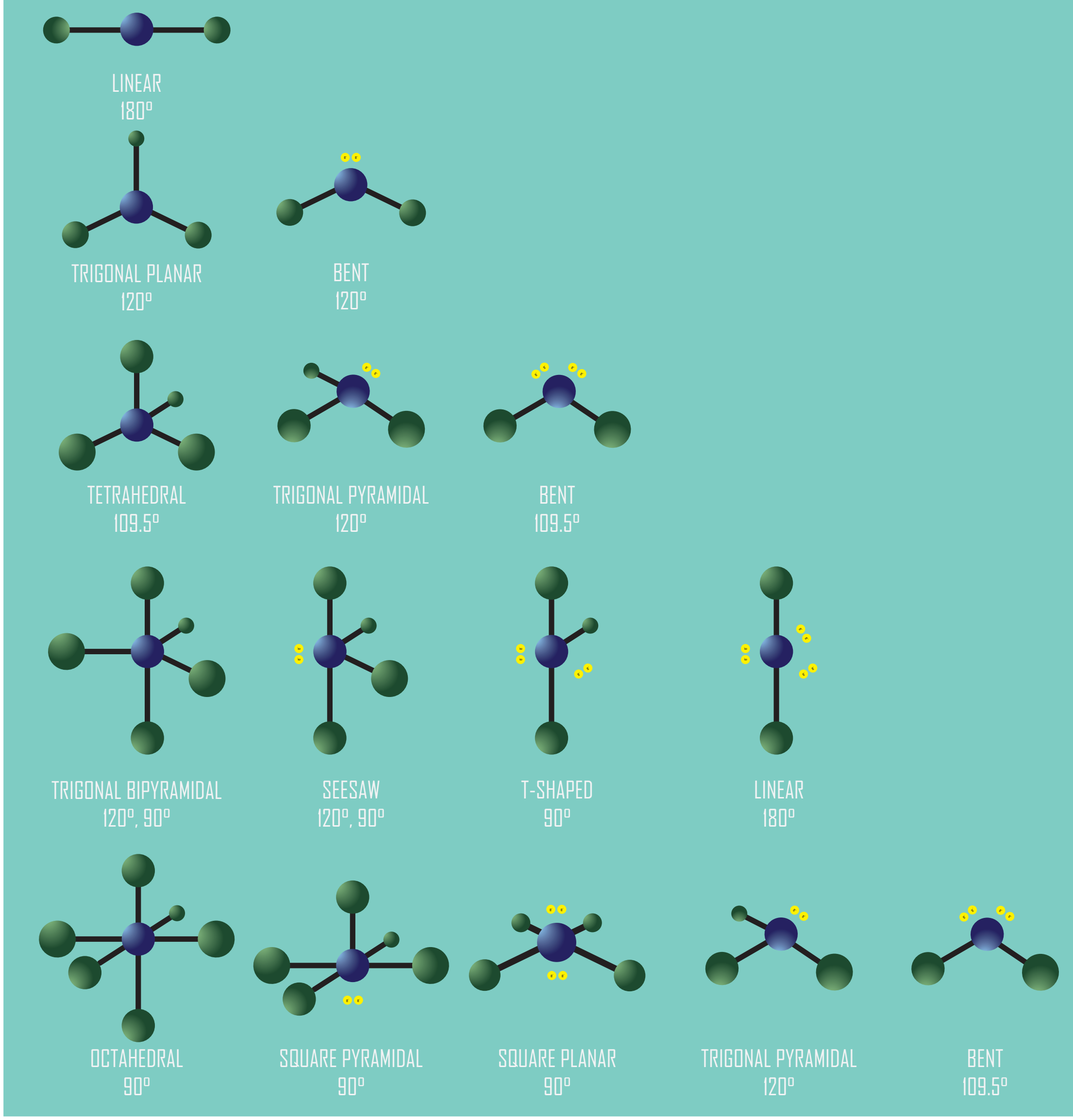
Remember, these are probabilities; the darker the area the higher the probability that an electron will be located there



sp molecular orbital

BONDS

VSEPR GEOMETRY IDENTIFICATION



-VSEPR - Valence Shell Electron Pair Repulsion

-VSEPR is a theory for predicting the 3 dimensional shape and orientation of molecules

-It gives one the configuration and angle measurements for different molecules

-These are shown on the right

-The easiest way of remembering VSEPR geometries is by drawing pictures of them

-When drawing structures out with electron pairs, it can be best to first draw and understand what the electron domain geometry is. This will give you the angle measurements for the molecule. One can then find the actual geometry (the molecular geometry) by removing the non-bonding electron pair(s) and seeing what remains

ELECTROCHEMISTRY

STANDARD CONDITION CELLS

-Standard condition cells are a way to generate an electric current
-To setup it up, it requires two beakers of two different metal solutions
-One beaker will have an un-ionized metal while the other beaker will have an un-ionized metal
-The un-ionized metal solution will soon become ionized which will result in the extra electrons (the ones kicked out during ionization) to flow through the channel and into the ionized metal solution. As a result the ionized solution will soon become un-ionized
-In order to facilitate this flow of electrons and ensure that there is a balance of charges, there is also a salt bridge connecting the two beakers
-Calculating E_{cell}:

$$E^0_{cell} = E^0_{reduction} + E^0_{oxidation}$$

NONSTANDARD CONDITION CELLS

The equation for nonstandard condition cells is given by:

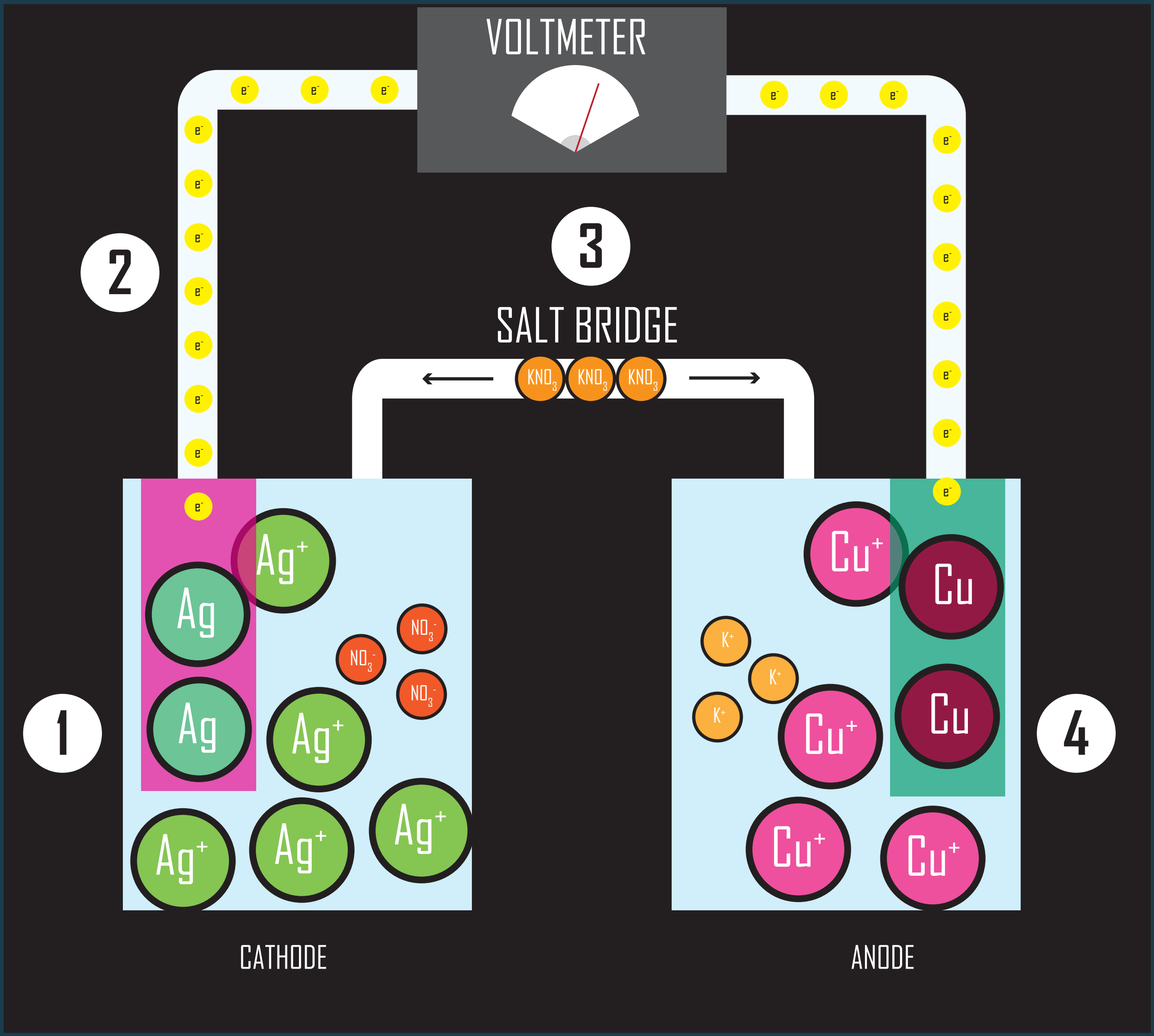
$$E_{cell}=E^\circ_{cell}-(RTnF)lnQ$$

Breaking it down:
E_{cell} is the actual cell potential
E°_{cell} is the standard cell potential
(RTnF)
R is the constant of 8.31 J/mole K
T is the temperature in kelvin
n is the number of moles the electrons transferred
F is Faraday's constant which is 96,485 C/mole e-
Q is the reaction quotient

$$E_{cell}=E^\circ_{cell}-(RTnF)lnQ$$

ELECTROCHEMISTRY

STANDARD CONDITION CELL



1) The silver atoms become silver ions releasing electrons that generate a current. The electrode loses silver atoms that go into the solution as ions. As a consequence, the mass of the silver electrode decreases

3) As a result of the increase in silver ions, compounds in the salt bridge disassociate to balance the ions in either solution

2) The electrons follow through to the anode, the other side of the cell

4) The electrons that reach the anode will cause in the copper ions in the solution to become copper, increasing the mass of the copper electrode

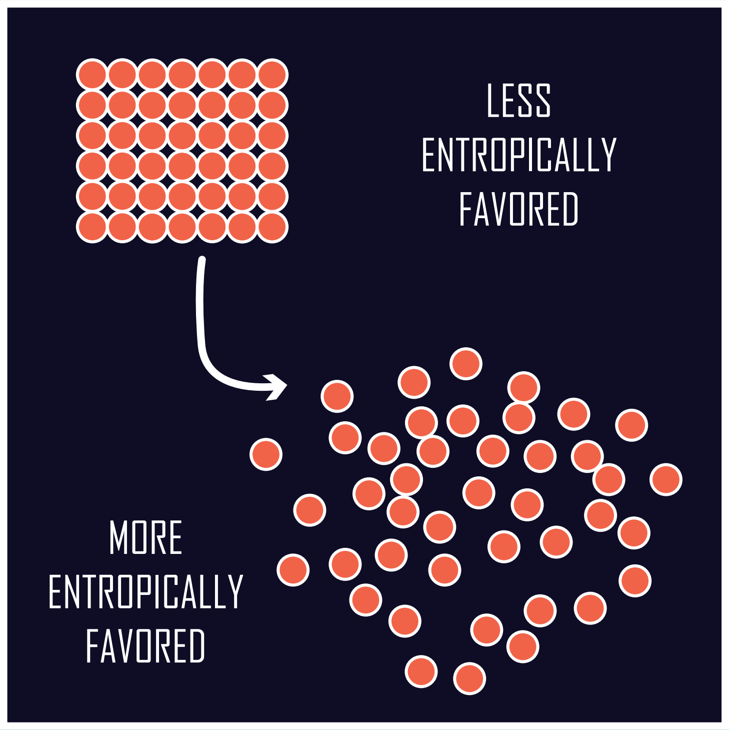
THERMODYNAMICS

ENTROPY (ΔS)

-Entropy refers to the **amount of disorder** or "chaos" in a system

-While it may seem odd, entropy (or disorder) is a favorable trait of a system to have

-As a result, one can assume that gases are more entropically favorable than solids



FREE GIBBS ENERGY (ΔG)

Free Gibbs Energy deals with thermodynamic favorability

$$\Delta G = \Delta H - T\Delta S$$

$$\Delta G = \Delta G^\circ + RT\ln Q$$

-Free Gibbs Energy is calculated by the equation: $\Delta G = \Delta H - T\Delta S$

-To be thermodynamically favorable, ΔG needs to be negative

-Entropy is favorable in a reaction => positive ΔS

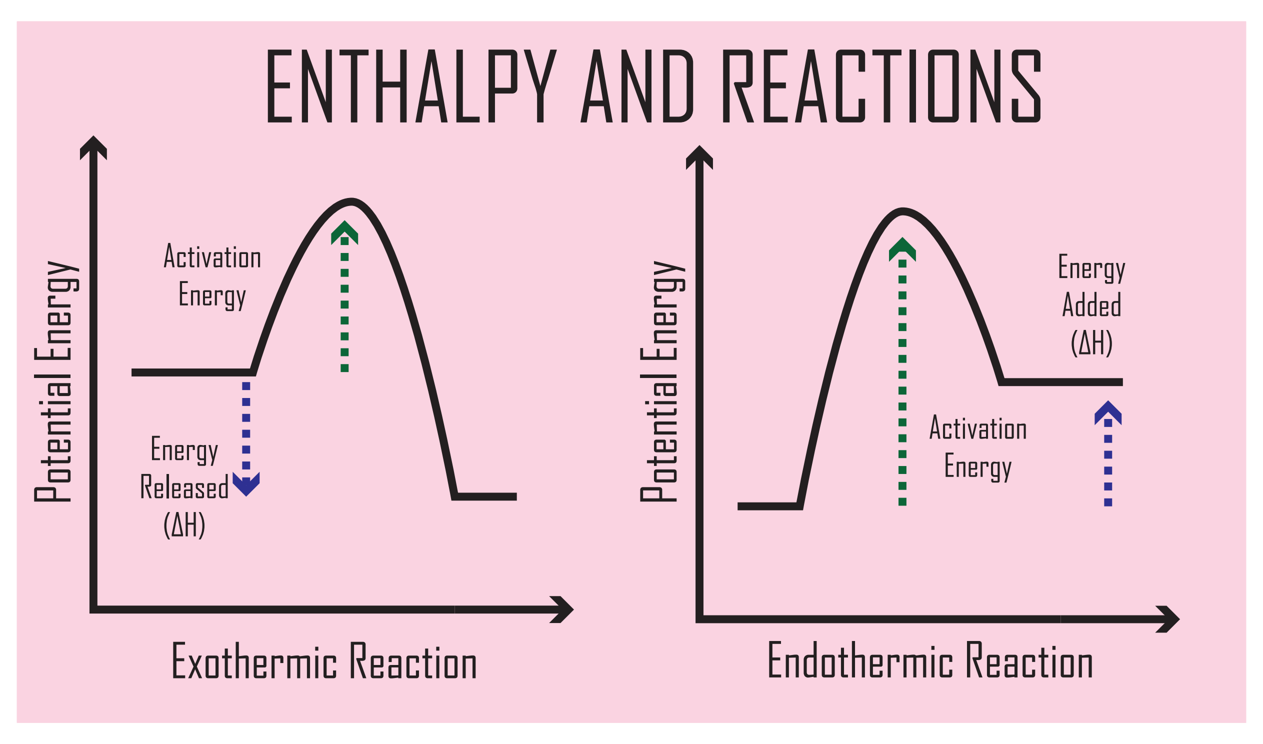
-Enthalpy is favorable when energy is lost => negative ΔH

-Will the reaction occur under the following conditions?

- -Positive ΔH and positive ΔS - one of the conditions is favorable
- -Positive ΔH and negative ΔS - neither condition is favorable
- -Negative ΔH and Positive ΔS - both conditions are favorable
- -Negative ΔH and negative ΔS - one of the conditions is favorable

ΔG° is the standard free state energy change
R is 8.314 J mol^{-1} K^{-1} or
T is the temperature in Kelvin
Q is the equilibrium constant at the given temperature

ENTHALPY (ΔH)



-Enthalpy refers to the heat change in a system and is represented by the symbol “ΔH”.

-Exothermic Reaction - this is when the amount of energy needed to form the products is less than the energy that is released when the reactants are broken. This means that overall the reaction gives off energy. When this is the case, ΔH will be negative.

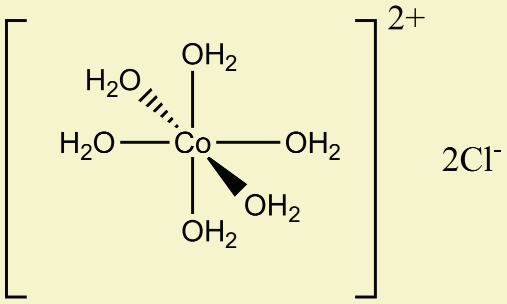
-Endothermic Reaction - this is when the amount of energy needed to form the products is more than the energy that is released when the reactants are broken. This means that the reaction takes in energy. When this is the case, ΔH will be positive.

Activation Energy - the amount of initial energy needed for the reaction to occur/start

The figure above is a diagram of the above terms

TRANSITION METALS

COORDINATION COMPLEXES



-While we previously stated that metals bond by using metallic bonding, they can also bond in other ways

-In coordination complexes, the metal atom is in the center of the structure and the various other atoms extend out from it (which are called “ligands”)

-Coordination complexes also rely heavily upon symmetry

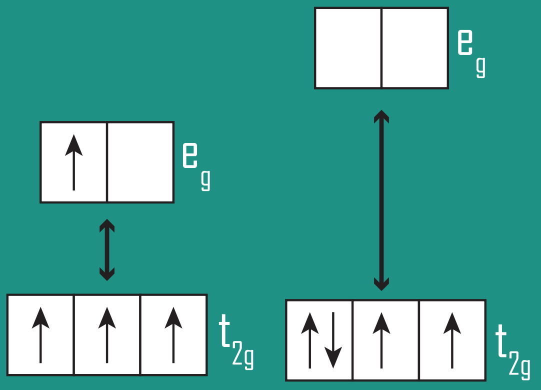
-The **coordination number** is the number of ligands attached to the metal

-Nomenclature/mono/polydentate

  -Compounds that end with “ide” end with “o”

    -Bromide becomes “Bromo”

CRYSTAL FIELD THEORY AND D-ORBITALS



-Coordination complexes have a special configuration of their d-orbital electrons

-Ions are assumed to be points

-These ionic points will thus cause greater electron repulsion in certain orbitals

Crystal Field Splitting -

  -Weak Field Ligand: a complex that maximizes the number of unpaired electrons; in turn the electrons are said to have **high spin**

  -Strong Field Ligand: a complex that minimizes the number of unpaired electrons; in turn the electrons are said to have **low spin**

-The difference in the gap between t_{2g} and e_g is caused by the size of the oxidation state of the attached ligands

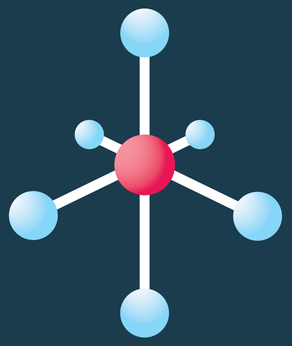
  -A spectrochemical scale organizes this from weak to strong ligands

  $I^- < Br^- < Cl^- < SCN^- < F^- < OH^- < ox^{2-} < ONO^- < H_2O < SCN^- < EDTA^{4-} < NH_3 < en < NO_2^- < CN^-$

-t_{2g} and e_g stand for different types of d-orbitals; t_{2g} represents the d-orbital with repulsions (with ligand) while e_g represents the ones that don’t

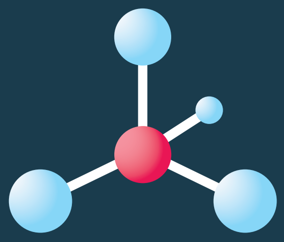
-The jumping of electrons falls within the spectrum of visible light, which gives the coordination complexes the vibrant colors they are often associated with

CRYSTAL FIELD THEORY AND GEOMETRIES



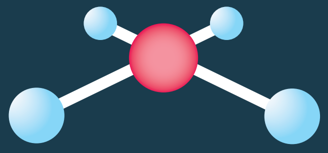
OCTAHEDRAL

6



TETRAHEDRAL

4



SQUARE PLANAR

4

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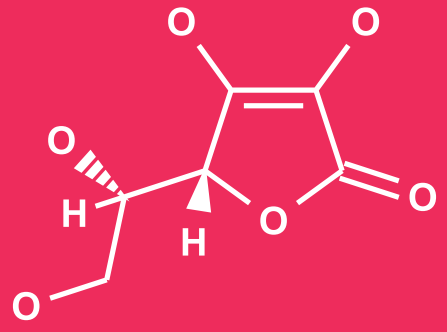
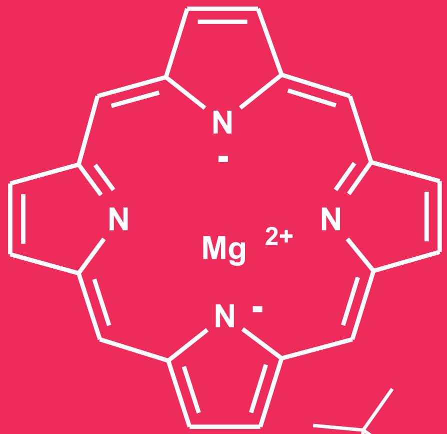
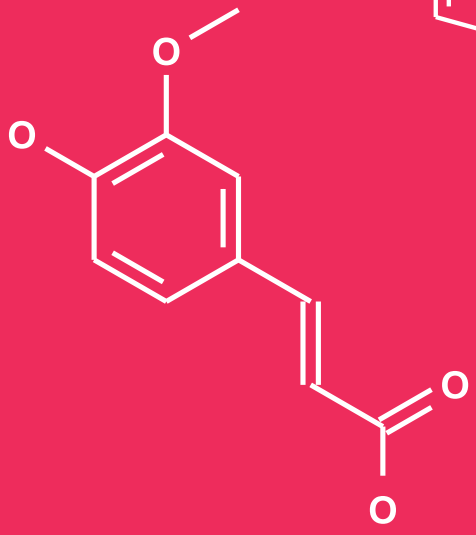
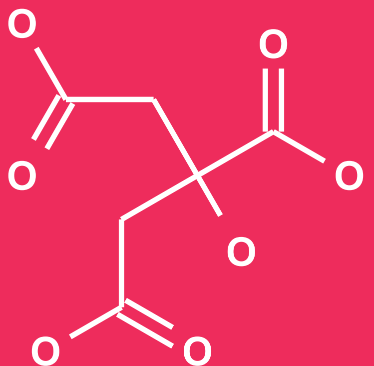
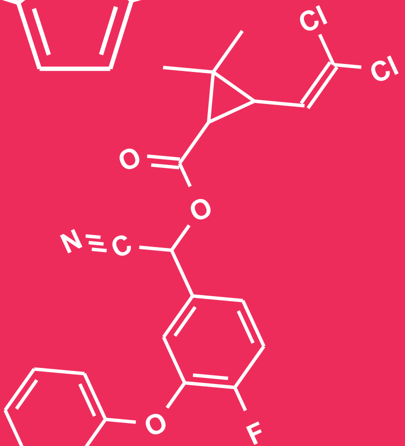


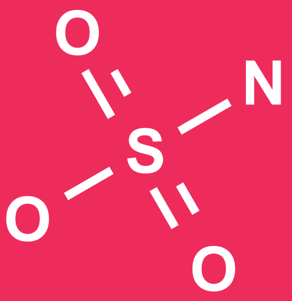


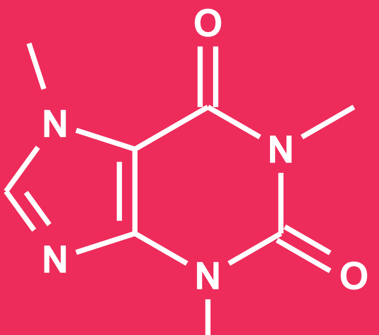


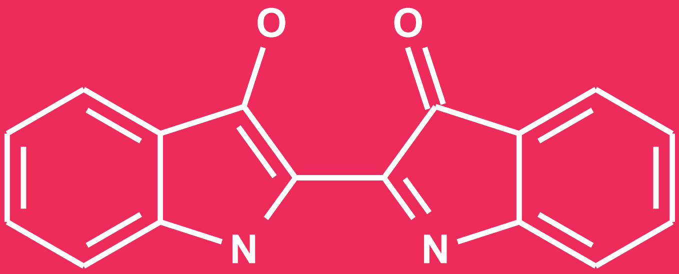




MEDICINAL CHEMISTRY







STAGES OF DRUG DEVELOPMENT

THE DRUG DEVELOPMENT PROCESS

Here are the steps of a possible drug development scenario. These steps will be discussed in further detail later on but for now this is a broad overview of the process.

BEGINNING

-In the beginning, scientists utilize computers (in silico) to help speed up their process. They begin by choosing what information they have and go from there:

1) Structure based screening - this is used when the structure of protein or receptor site is known. Sets of ligands are tested at the protein's binding site and binding affinity and thermodynamic favorability are calculated.

2) Ligand based screening - ideal if you have a chemical compound in mind that you would like to work with or a compound derived from nature that showed biological activity. It is also used when the receptor site that the ligand will bind with is unknown. Similar compounds can be found using libraries online (such as the ZINC library) and similarity can be calculated by using a Tanimoto Score

IDENTIFYING THE TARGET

-Scientists need to determine what to focus their efforts on
-They need to identify that their biological target (a gene or protein) has a possible role in the disease that they are trying to remediate
-If there are not any models for the protein in a research database, X-ray crystallography may need to be used to create a model of the protein from experimental data
-They may also need to figure out which site of the protein is most favorable for their desired outcome
-Target validation also needs to occur to ensure that the target they are focusing on has the potential to be adjusted to result in medicinal effects
-They can also see if the protein has good druggability, or the ability or potential to bind well with a ligand
-After ensuring their target, screenings can be carried out

HIT-TO-LEAD

Once scientists are able to identify their target, screenings can occur to try and identify which ligands show the most promise based off of binding affinities as well as other chemical factors such as the molecule's polar surface area and the molecule's ability to donate or accept a hydrogen bond
Once the hundreds of thousands (if not millions) of ligands have been filtered to a much more feasible number (e.g. around a 100), structure activity relationships need to be done to see what are the critical moieties in the structure for interaction with the protein and what affect adding or subtracting certain ligands have on protein interaction
SAR studies also need to be done to identify the critical moiety (pharmacophore) of the ligand compounds

OPTIMIZATION/TESTING

-After desirable lead compounds have been chosen, scientists need to figure how to adjust or optimize them for various purposes
-They will also test the ligands by conducting "in vitro" or assay screenings on cell cultures and if the ligand is promising enough, "in vivo" tests on animals
-There is also a big gap between theoretical calculations done on the computer and experimental results
One of the reasons that account for this is the fact that in order to perform computer screening in a practical amount of time, receptor models are oftentimes static and do not represent the accurate dynamic configuration of a receptor that is found
-Other problems may include that the compound may bind very well but may cause unwanted side effects or the compound may be too costly or difficult to synthesize for the market

FURTHER TESTING, TRIALS, & PRODUCTION

-Once this stage has been reached, significant computational testing has been done as well as some experimental testing and has proved to be favorable. By now just a handful of compounds have been identified as worthy enough to continue on testing, specifically clinical testing.
-Even after rigorous testing, 90% of the candidates selected for clinical testing do not pass
-In the end, several years would have been spent researching, developing, and testing the drug and close to a billion dollars have been spent to develop the drug

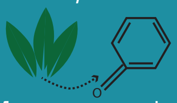
FINDING LEAD COMPOUNDS

TRADITIONAL MEANS

Traditional Knowledge

- Traditional knowledge is vital for discovering new medicines as it can oftentimes be a launch pad for discovering new treatments

- Some of these sources may include the Ayurveda, Chinese medicine, Arabian medicine, or even folklore



- Pharmacognosy

- Pharmacognosy is deriving drugs from compounds from plants

-Other sources in nature for potential drug candidates include microorganisms, marine life, animal sources, and even venom (e.g. from snakes or spiders)

RATIONAL DRUG DESIGN

Functional Groups/Bioisosterism - The idea of functional groups is grounded in the principle that specific chemical groups will exhibit specific biological properties regardless of the molecular structure they are in.

Fragment Based Drug Discovery - Researchers use nuclear magnetic resonance spectroscopy (NMR) to find out and see how a ligand binds to a protein

COMPUTATIONAL METHODS

-Through technological advancements and computational methods, the drug discovery process has rapidly been sped up

-Scientists can now employ computers (sometimes referred to as "in silico" methods derived from the fact that silicon is used in computer chips) to help get a jumpstart at sifting through and finding promising drug candidates

-Instead of relying on luck or previous knowledge, once they have identified a viable protein binding site ("target identification) scientists can now sift through libraries of chemical compounds (oftentimes with tens of millions of compounds) to find promising ones (ligands) that would likely show strong affinity for a given protein

-This is known as High Throughput Screening

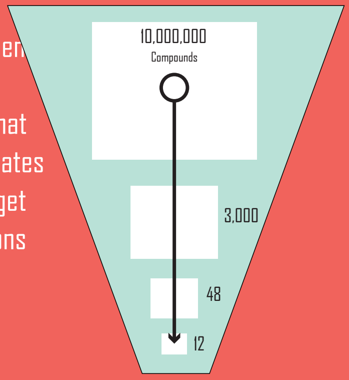
There are various other methods used to help facilitate the discovery process. These include:

-Homology Models, Molecular Docking, QSAR, Pharmacophore Screening

-While this process may seem miraculous, it does have its limitations. They are primarily due to:

-Inaccuracy with computational models and methods

-Limited computational power due to limited hardware capabilities.



REPRESENTATION OF THE SCREENING PROCESS

OTHER APPROACHES

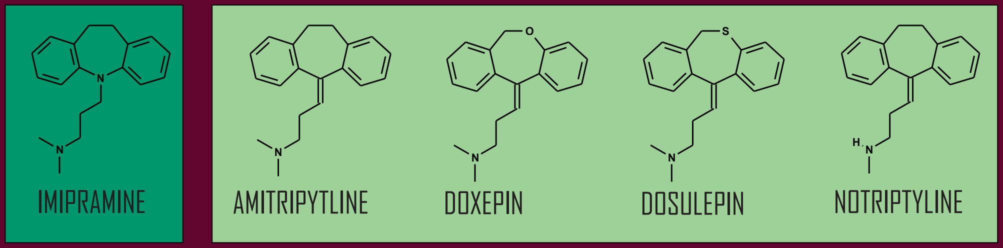
"MeToo" Drugs

Sometimes drug companies will take an already known and successful drug and make small changes to it. By doing this, these companies will be able to commercially synthesize and sell the drug because it will be considered a "new" drug and won't infringe on existing patents, even if their modifications result in hardly any change of the effect of the drug.

Drug Repositioning

Existing drugs are investigated for use in new ways. This will be discussed in more detail later.

A VISUALIZATION OF "ME TOO" DRUG DEVELOPMENT



The original drug

"Me Too" Variations

CHEMICAL TESTING

IMPORTANCE AND REASONS

-So now we have identified a whole slew of potential lead compounds either via computational methods or pharacognosy, but how do we identify which compounds truly show promise and which ones are merely false hopes?

-There are various requirements that a drug must pass through before a drug is sent to market

-These requirements are vital in the development of the drug as, without them, major safety problems can go overlooked causing great harm to thousands of people

-This can be seen with the case and catastrophe of the children of Thalidomide

-So why might a once promising drug candidate become rejected during the development process? Here are some major reasons:

SAFETY

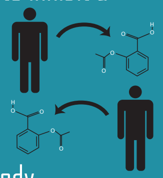
Therapeutic Index

-Refers to a drug's safety; the ratio of desirable versus undesirable effects

-Safety of drug metabolites (compounds made through body and drug interaction)

IC_{50} - refers to the amount of substance needed to inhibit a process by 50%

KI - inhibition constant



Pharmacodynamics

-Refers to how a drug interacts with a person's body

ACTIVITY

-Lipinski's Rule of 5

-Guidelines for how well a drug will work or how well it will be absorbed

-It is used as a rule of thumb, specifically with how well a particular compound may work as an oral drug

Water Solubility

-This can be predicted by measuring logP

Similarly, **Jorgenson's Rule of Three** is another rule of thumb on the absorption of a drug

ADME

ADME stands for absorption, distribution, metabolism, and excretion

-Refers to how a person's body interacts with the drug or pharmacokinetics

BIOLOGICAL TESTING

"In vitro" testing -- "in vitro" testing refers to tests done with assays

"In vivo" testing -- refers to testing with live animals

These are tests in increasingly more complex organisms to ensure that the functionality of the compound in question remains experimentally and when put up against organisms that are more similar to humans (this is particularly true in in vivo testing)

MISC.

-The ligand may be very promising and bind very well to a protein

-However, if the drug is too difficult to synthesize or is not commercially feasible it may be rejected

-This has happened with multiple drugs over the years; while one ligand may have a stronger affinity, it is too difficult to feasibly synthesize so a chemical with an inferior affinity but with a greater ease of production is chosen

INSIGHTS

STRUCTURE-ACTIVITY RELATIONSHIPS

-Structure-activity relationships are one of the most important tools a medicinal chemist has, and they rely on the principle that the structure of a compound determines its functionality

-Structure-activity relationships can be useful when conducting a virtual screening

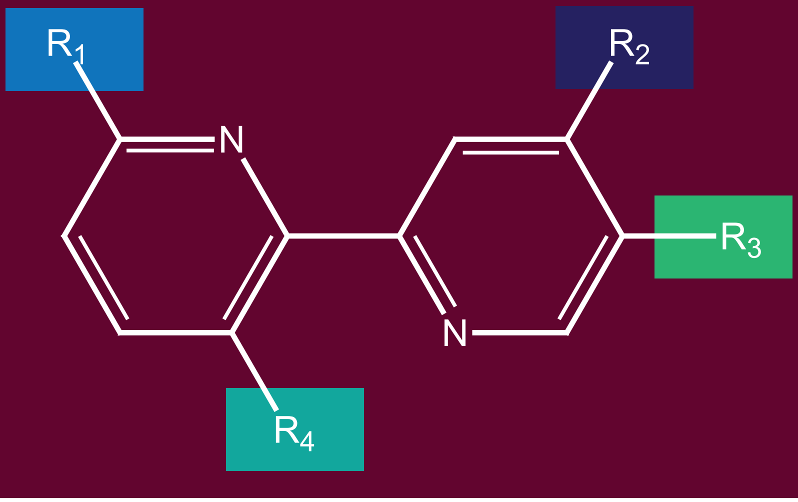
-The hit series of ligands can be analyzed to see which groups the hit ligands have in common and this can act as the "backbone" structure in guiding modifications and narrowing of the promising ligands

-However, SAR is a very helpful tool in the lead optimization stage, where it is most used

-SAR is employed by swapping out different groups with structures with known properties (lipophilicity, high metabolic rate, etc.)

-They help scientists find patterns, better visualize a given compound and what aspects of the compound are favorable and are interacting well with the target

-SAR also allows scientists to hypothesize and identify which physiochemical properties of the ligand that are more critical than others (e.g. if they swap out methyl group for a trifluoromethyl, and there is not a significant change in the favorability of the interaction, electronic properties may not play a huge role, specifically in that part of the molecule's interactions with the protein. However, if they fused two benzene rings together and created a naphthalene ring, and there was a sizeable favorability change in the protein interaction, they can hypothesize that for this receptor steric properties are significant.



QSAR

QSAR - Quantitative Structure-Activity Relationships

QSAR is a type of structure activity relationship where molecular descriptors or molecular characteristics are taken from a set of compounds and the data used helps to make predictions about the favorability of certain compounds. It is structure optimization based on quantitative data of physiochemical properties. For example, if one has data for a set of compounds on logP, a characteristic of water solubility, one can then see how adding different groups will change the water solubility of the compounds and seeing patterns in this data can help elucidate which groups are most beneficial to this and allows one to make predictions on novel compounds to test. This helps speed up the drug development process and permits one to see how multiple physiochemical properties are affected when introducing a certain functional group.