General Chemistry: A Guided Review for Study

This review is, by no means, intended to be a completely comprehensive review of general chemistry. This guide is intended to serve as a *reminder* of selected topics that must be reviewed before beginning organic chemistry. You will be quizzed on your understanding and comprehension of the topics listed in the "Review of General Chemistry Topics," and this study may help to refresh your memory of those topics. If you find that the level of detail here does not refresh your memory of a topic, you should look up that topic in a general chemistry text for more detail.

Chemical Equilibrium

Law of Mass Action

For a reaction: $j\mathrm{A} + k\mathrm{B} \rightleftharpoons k\mathrm{C} + m\mathrm{D}$
the law of mass action is represented by the following equilibrium expression:
$K = \dfrac{[C]^l[D]^m}{[A]^j[B]^k}$, where *K* is the equilibrium constant.
The reaction quotient, *Q* is obtained by applying the law of mass action, but using initial concentrations instead of equilibrium concentrations.
For (1) $Q = K$, system is @ equilibrium $\therefore$ no shift will occur; (2) $Q>K$, system shifts left; (3) $Q<K$, system shifts right.

Significance of the Magnitude of *K* (K_c; K_p; K_a; K_w, K_{sp})

K_c is the equilibrium constant and the subscript *c* indicates that it is in terms of concentration, when the reaction occurs in the gas phase, the equilibrium constant is K_p where *p* indicates that it is in terms of pressure (refer to a physical chemistry text for a discussion on activities and standard states). For dilute solutions, K_c and K_{eq} are used interchangeably. K_a refers to the equilibrium constant for acid dissociation reactions, K_b refers to the equilibrium constant for base dissociation, and K_w refers to the autoionization of water: $H_2O(l) \rightleftharpoons H^+(aq) + OH^-(aq)$. For $K_w = 1.0 \times 10^{-14} = [H^+][OH^-]$, then if $[H^+] > 10^{-7}$ then the solution is acidic, and if $[OH^-] > 10^{-7}$ then the solution is basic. By applying LeChâtelier's principle: pure water is a system in equilibrium with its ions, and adding either acid, H^+, or base, OH^-, will cause the equilibrium to shift to the left, toward neutral water, that is, water ionization is inhibited in acidic or basic solutions. We use a logarithmic scale known as the pH scale (standing for the negative of the **p**ower of the **H**ydrogen ion concentration), defined by: $\mathrm{pH} = -\log_{10}[H^+]$, and if we take the $-\log_{10}$ of both sides of the previous equation, then we get $\mathrm{pH} + \mathrm{pOH} = \mathrm{p}K_w = 14.00$, which is temperature dependent.

Summary of equilibrium constant values:

As the value of $K_c \uparrow$, $\dfrac{[products]}{[reactants]} \uparrow$	As the value of $K_p \uparrow$, $\dfrac{[products]}{[reactants]} \uparrow$	As the value of the $K_a \uparrow$, the acid strength $\uparrow$	As the value of the $K_{sp} \downarrow$, the solubility $\downarrow$

Relationship between *K* and Spontaneous Reactions

Gibbs free energy (G) is a measure of reaction spontaneity:
$G = H - TS$ (H = enthalpy, T = temperature, and S = entropy) and $\Delta G = \Delta H - T\Delta S$
$\Delta G = 0$ condition allows reversible or equilibrium processes to be described.
As a reaction proceeds, the free energy that guarantees its spontaneity is expended, and eventually the system will reach equilibrium.

When equilibrium has been attained ($\Delta G = G_P - G_R = 0$ is the equilibrium condition, and $\Delta G < 0$ at constant T, P results in a spontaneous process), we have:

$$\Delta G = G_P - G_R = 0 = \Delta G^\circ + RT\ln Q_{eq}, \text{ where } Q_{eq} = K$$

and by substituting *Q* (at equilibrium) for K:

$$\Delta G^\circ = -RT\ln K \quad \text{or} \quad K = e^{\frac{-\Delta G^0}{RT}}$$

At a fixed temperature, *K* is truly a constant, since ΔG° depends only on *T*, the nature of the system, and the definition of the standard state (see "standard heats of formation"). For (1) $\Delta G^\circ = 0$, K = 1; (2) $\Delta G^\circ < 0$, K > 1; (3) $\Delta G^\circ > 0$, K < 1

Acid-Base Equilbria: Strong and Weak Acids and Bases

Strong acids are strong electrolytes which, for practical purposes, are assumed to ionize completely in water. Most of the strong acids are inorganic acids: hydrochloric acid, nitric acid, perchloric acid, and sulfuric acid (not that H_2SO_4 is a diprotic acid, thus it will have two dissociation constants). Most acids are weak acids, which ionize only to a limited extent in water. At equilibrium, aqueous solutions of weak acids contain a mixture of nonionized acid molecules, H_3O^+ ions, and the conjugate base according to the acid dissociation constant, K_a.. Examples of weak acids include: hydrofluoric acid, acetic acid, and the ammonium ion. So, when calculating the concentration of HF in a solution, one has to account for the following condition: $HF(aq) \rightleftharpoons H^+(aq) + F^-(aq)$, $K \equiv K_a = 7.0 \times 10^{-4}$. Notice that the equilibrium constant is a unitless number (it is a ratio).

The limited ionization of weak acids is related to the equilibrium constant for ionization. Like strong acids, strong bases are strong electrolytes (examples are metal hydroxides: NaOH, e.g.), and weak bases are weak electrolytes (NH_3, e.g.). Nearly all weak bases act as bases not by donating OH^- to the solution, but by splitting or *hydrolyzing* water to produce OH^-. Consider ammonia: $NH_3(aq) + H_2O(l) \rightleftharpoons NH_4^+(aq) + OH^-(aq)$, $K \equiv K_b = 1.79 \times 10^{-5}$.

Chemical Thermodynamics

Relationship between Enthalpy Change, ΔH_{rxn} and Heat Flow, q_{rxn}

For an isobaric process, $\Delta H = q_p$

The change in enthalpy of a system has no easily interpreted meaning except at constant pressure, where ΔH = heat.

For a chemical reaction the enthalpy change is given by the equation:

$\Delta H = H_{products} - H_{reactants}$

At constant pressure exothermic means ΔH is negative; endothermic means ΔH is positive.

The "heat of reaction" is the enthalpy change per mole.

The origin of the heat of a reaction can be traced to the difference in bond energies (D_0) between the product and reagent molecules. Bond breaking is endothermic, so bond enthalpies are positive. Chemical reactions usually absorb or release heat: energy must be absorbed to break a chemical bond & energy is released when a chemical bond forms (see "bond energies" below).

Comparing Thermochemical Quantities

	definition	SI units	type
temperature	hotness/coldness property that controls direction of heat flows	K	intensive property
thermal energy	energy due to molecular motions	J	extensive property
heat	transfer of thermal energy due to a temperature difference	J	process
enthalpy	adjusted thermal energy	J	extensive property

Standard Heats of Formation, ΔH_f°

Definitions of Standard States:

For a gas the standard state is a pressure of exactly 1 atm. For a substance present in a solution, the standard state is a concentration of exactly 1 *M* at an applied pressure of 1 atm. For a pure substance in a condensed state (liquid or solid), the standard state is the pure liquid or solid. For an element the standard state is the form in which the element exists (is most stable) under conditions of 1 atm and the temperature of interest (usually 25°C).

The *standard enthalpy of formation* (ΔH_f°) of a compound is defined as the change in enthalpy that accompanies the formation of 1 mole of a compound from its elements with all substances in their standard states.

Key Concepts for Doing Enthalpy Calculations:

When a reaction is reversed, the magnitude of ΔH remains the same, but the sign changes. When the balanced equation for a reaction is multiplied by an integer, the value of ΔH for that reaction must be multiplied by the same integer. The change in enthalpy for a given reaction can be calculated from the enthalpies of formation of the reactants and products: $\Delta H = \Sigma\Delta H_f^\circ{}_{(products)} - \Sigma\Delta H_f^\circ{}_{reactants)}$. Elements in their standard states are not included in the $\Delta H_{reaction}$ calculations. That is, H_f° for an element in its standard state is zero.

Hess's Law

Because the energy of a given element or compound (see "chemical bond energies") at a given pressure and temperature is an intrinsic property of that substance, the heats of reaction for reactions involving one or more of he same elements or compounds are related to each other, as first shown by Hess in 1840. *Hess's law of constant heat summation states that the heat of any reaction that can be obtained by adding other reactions is given by the same sum of the heats of those other reactions.* That is, if reaction (a) + reaction (b) = reaction (c), then $\Delta H_a + \Delta H_b = \Delta H_c$; stoichiometric multipliers that adjust the amounts of reactions to add also apply to the ΔH relation. The heat of a reaction carried out backward (products → reactants) is the negative of the forward heat. Hess's law implies that we do not have to measure the heat of every possible reaction as long as we know the heats of some component reactions. The standard reactions that chemists have chosen are the formation reactions, those in which a compound is formed from its constituent elements in their most stable states at 1 atm and 298 K.

Chemical Bond Energies (D_0)

We can obtain information about the strength of a bonding interaction by measuring the energy required to break the bond, the bond energy (D_0). In an exothermic process ($q < 0$) the bonds in the products are stronger (on average) than those of the reactants (vast majority of reactions). That is, more energy is released in forming the new bonds in the products than is consumed in breaking the bonds in the reactants. The net result is that the quantity of energy Δ(PE) is transferred to the surroundings through heat. Many endothermic ($q > 0$) reactions are also known To systematize the tabulation of experimental reaction heats, the results are reported as enthalpy changes at 1.00 atm pressure and 298.15 K (NTP) per mole of reaction, ΔH°_{298}, in either kilocalories per mole or kilojoules per mole. For example, the bond energy of the C – H bond, D_0(C – H), is taken as an average of the four bonds in $CH_4(g)$, and differs slightly from that in any individual bond in CH_4 or in other molecules possessing that bond. In molecules such as benzene (C_6H_6), a further complication occurs because of delocalized π bonding, which makes the molecule more stable than one would predict based on the bond energies corresponding to a single Lewis structure resonance form. The difference between the predicted and experimental heats of formation of molecules such as benzene is called the resonance energy. When estimating ΔH from bond enthalpies, one should adopt the following strategy: imagine reaction as a) dissociation of reactants into atoms, b) recombination of atoms into products. (1) Add enthalpies for all product bonds. (2) Add enthalpies for all reactant bonds. (3) ΔH is approximately the difference between the product and reactant bond enthalpies.

Summary of Enthalpy of Reaction:

Reaction type:	exothermic	endothermic
heat is:	released	absorbed
reaction vessel temperature:	rises	falls
enthalpy change is	negative	positive
number or strength of bonds:	increases	decreases

Chemical Kinetics

Reaction Rate and the Reaction Rate Constant, *k*

Rate is expressed in the units of moles per liter per second ($mol \cdot L^{-1} \cdot s^{-1}$) or molarity per second ($M \cdot s^{-1}$).

$$rate = \frac{decrease\ in\ concentration\ reactants}{time} = \frac{increase\ in\ concentration\ products}{time}$$

In general, for a reaction: aA + bB → cC + dD,

$$rate = -\frac{1}{a}\frac{\Delta[A]}{\Delta t} = -\frac{1}{b}\frac{\Delta[B]}{\Delta t} = \frac{1}{c}\frac{\Delta[C]}{\Delta t} = \frac{1}{d}\frac{\Delta[D]}{\Delta t}$$

Factors Affecting Reaction Rate: (1) reaction concentration, (2) temperature, (3) medium, (4) catalysts

Differential and Integrated Rate Laws

For nearly all forward, irreversible reactions, the rate is proportional to the product of the concentrations of the reactants, each raised to some power. For a general reaction of the type:

$$aA + bB \rightleftharpoons cC + dD$$

the rate is proportional to $[A]^x$ $[B]^y$, that is:

$$rate = k[A]^x[B]^y$$

This expression is the rate law for the general reaction above, where k is the rate constant. The exponents x and y are called the orders of reaction; x is the order with respect to A and y is the order with respect to B. These exponents may be integers, fractions, or zero, and *must be determined experimentally*. The overall reaction order is the sum of all exponents, in our example, x+y.

Experimental Determination of Rate Constants

The values of *k*, x, and y in the rate law equation (rate= $k[A]^x[B]^y$) must be determined experimentally. One method is to measure the rate initially as a function of the initial concentration of the reactants A and B (called *the initial rate method*). Another way is to collect concentration data over time and solve the integrated form of the rate equation by setting the general rate law equal to the rate expression as a function of disappearance of product and then applying calculus.

Arrhenius Energy of Activation, E_a

The dependence of the rate constant of a reaction on temperature can be expressed by the following equation, known as the *Arrhenius equation* :

$$k = Ae^{-\frac{E_a}{RT}}$$

where *A* represents the collision frequency (from the collision theory of chemical kinetics), E_a is the activation energy of the reaction (kJ/mol), *R* the gas constant (8.3145J/K·mol), *T* the absolute temperature, and *e* the base of the natural logarithm scale. A plot of ln *k* versus 1/T (the rate constant at various temperatures must be collected experimentally) whose slope is *m* is equal to $-E_a/R$ and whose intercept *b* with the ordinate (the *y* axis) is ln A from the equation:

$$\ln k = \left(-\frac{E_a}{R}\right)\left(\frac{1}{T}\right) + \ln A$$

Chemical Reaction Mechanisms

The mechanism of a reaction is the actual series of steps through which a chemical reaction occurs. Knowing the accepted mechanism of a reaction often helps to explain the reaction's rate, position of equilibrium, and thermodynamic characteristics. A theoretical mechanism can be supported by experimental kinetic data, not the other way around. Kinetic data can support mechanisms, but proposed mechanisms must agree with experimental data if they are to be a theoretical framework on which to base further explanation of events. For an overall reaction of the type:

$$A_2 + 2B \rightleftharpoons 2AB$$

a possible mechanism would be the following two step process:

Step 1: $A_2 + B \rightarrow A_2B$ (slow)
Step 2: $A_2B + B \rightarrow 2AB$ (fast)

Note that these two steps add up to the overall (net) reaction, a necessary requirement for a plausible mechanism. A_2B does not appear in the overall (net) reaction because it is neither a reactant nor product, but is an intermediate. Reaction intermediates are often difficult to detect, but can be supported through kinetic data (as mentioned earlier). For example, suppose that the rate law of the above reaction was: rate = $k[A_2][B]$, the above mechanism would be plausible. The slowest step in a reaction mechanism limits the overall rate of a reaction, and this step is often called the rate-limiting step or the rate-determining step.

Oxidation-Reduction (Redox) Reactions

Reactions involving transfer of electrons between species

The law of conservation of charge states that an electrical charge can be neither created nor destroyed. Thus, an isolated loss or gain of electrons cannot occur; oxidation (loss of electrons – OIL) and reduction (gain of electrons – RIG) must occur simultaneously, resulting in an electron transfer called a redox reaction. An oxidizing agent causes another atom in a redox reaction to undergo oxidation, and is itself reduced. A reducing agent causes the other atom to be reduced, and is itself oxidized.

Assigning oxidation numbers:

(1) The oxidation number in free elements is zero. (2) The oxidation number for a monoatomic ion is equal to the charge of the ion. (3) The oxidation number of each Group IA element in a compound is +1. The oxidation number of each Group IIA element in a compound is +2. (4) The oxidation number of each Group VIIA element in a compound is -1, except when combined with an element of higher electronegativity. (5) The oxidation number of hydrogen is +1 unless it is in compounds with less electronegative elements than hydrogen, and the oxidation

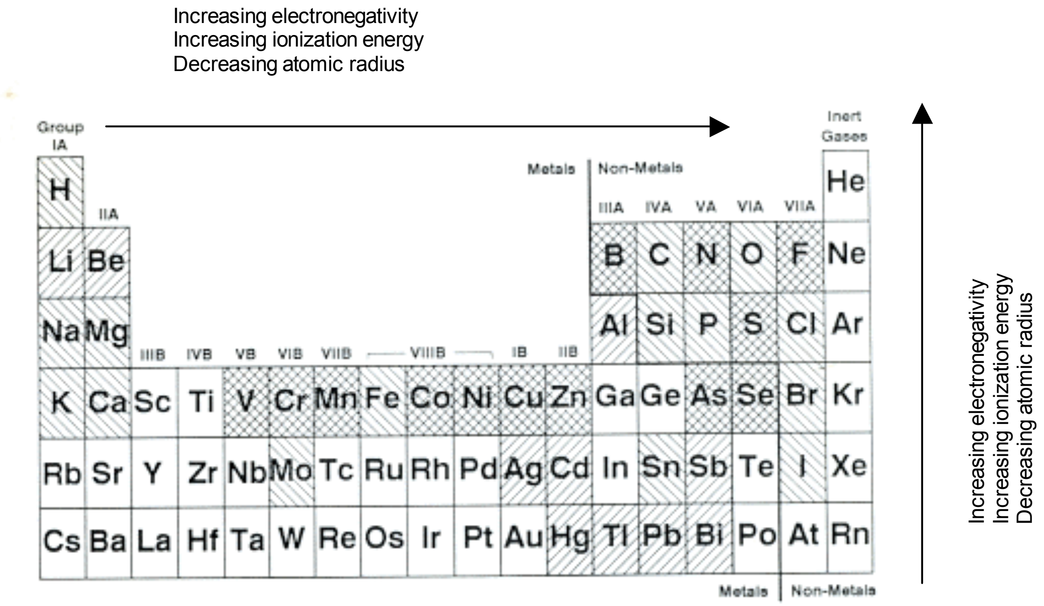
state will be -1. (6) In most compounds the oxidation number of oxygen is -2. The exception is in peroxides, or in compounds that such as OF_2 (fluorine is more electronegative than oxygen). (7) The sum of the oxidation numbers of all the atoms present in a neutral compound is zero. The sum of oxidation numbers of the atoms present in a polyatomic ion is equal to the charge of the ion.

The most common method for balancing the redox reactions is the half-reaction method, also known as the ion-electron method, in which the equation is separated into two half-reactions – the oxidation part and the reduction part. Each half-reaction is balanced separately, and the reactions are added together to give the complete, balanced, redox reaction.

Molecular and Ionic Structure

Periodic Properties

Note: the effective nuclear charge, Z_{eff} can explain all periodic trends as well as chemical properties.



1. Atomic Radii

The atomic radius of an element is equal to one-half the distance between the centers of two atoms of that element that are just toughing each other. In general, the atomic radius decreases across a period from left to right and increases down a given group; the atoms with the largest atomic radii will be located at the bottom of groups, and in Group I. The effective nuclear charge increases steadily across a period, and this causes the atomic radius to decrease.

2. Ionization Energy

The ionization energy (IE), or sometimes referred to as the ionization potential, is he energy required to completely remove an electron from a gaseous atom or ion.

Removing an electron from an atom always requires an input of energy (is endothermic). The first ionization energy is the energy required to remove one valence electron from the parent atom, the second ionization energy is the energy needed to remove a second electron from the univalent ion to form the divalent ion, and so on. Successive ionization energies grow increasingly large. Ionization energy increases from left to right as the atomic radius decreases. Moving down a group, the ionization energy decreases as the atomic radius increases. Group I elements have low ionization energies because the loss of an electron results in the formation of a stable configuration (octet).

3. Electron Affinity

Electron affinity is the energy change that occurs when an electron is added to a gaseous atom, and it represents the ease with which the atom can accept an electron. The stronger the attractive pull of the nucleus for electrons (effective nuclear charge, or Z_{eff}), the greater the electron affinity will be. Two sign conventions: (1) the more common one states that a positive electron affinity value represents energy release when an electron is added to an atom; (2) the other states that a negative electron affinity represents a release of energy.

4. Electronegativity

Electronegativity is a measure of the attraction an atom has for electrons in a chemical bond. The greater the electronegativity of an atom, the greater its attraction for bonding electrons. Electronegativity values are not determined directly (they are not experimentally measured; they are calculated values). The Pauling electronegativity scale is the most commonly used method, and ranges from 0.7 → 4.0 the most electronegative element, fluorine. Electronegativities are related to ionization energies in a directly proportional relationship.

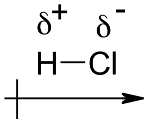
Covalent and Ionic Bonding

Classification of chemical bonds begins with identify two distinct types: ionic bonds and covalent bonds. In general (there is a much more accurate, but time consuming method for distinguishing between ionic and covalent bonds), the difference in electronegativity of two atoms involved in a bond must be ***greater than 1.7***. In a covalent bond, the electronegativity difference is considerably ***less than 1.7.***

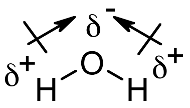
Polarity of Bonds and of Molecules

In ionic bonding, an electron from an atom with smaller ionization energy is transferred to an atom with a greater electron affinity, and the resulting ions are held together by electrostatic forces. In covalent bonding, an electron pair is shared between two atoms, although not necessarily shared equally: on average, the majority of the electron density will be concentrated on more electronegative of the two elements in a polar chemical bond. If the two atoms involved in a covalent bond have the exact same electronegativity, or the electronegativity values are very close (e.g., C – H), the bond is considered to be nonpolar. For polar bonds, the bond can be considered partially ionic and partially covalent due to the electronegativity difference between the two elements.

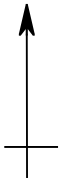
Polar bonds are represented in the following way:



A molecule with polar bonds may not be a polar molecule: the bond dipole moments may cancel each other out, resulting in a nonpolar molecule. Although a m9lecule with polar bonds need not be polar, a polar molecule must have polar bonds. A molecule with a net dipole moment is called polar because it has positive and negative poles. H_2O, for example is a polar molecule. See the illustration below for the notation of polarity (region of excess electron density corresponds to the arrow end, region of electron deficiency corresponds to the "positive" portion of the arrow.



polarity vectors for H_2O



net dipole moment for H_2O

Another important topic, intermolecular forces, will not be discussed. Weaker than intramolecular chemical bonds, intermolecular forces are of considerable importance in understanding the physical properties of many substances.

The following discussions concern covalent bonding...

Properties of Covalent Bonds

1. Bond Length

Bond length is the average distance between the two nuclei of the atoms involved in the bond. As the number of shared electron pairs increases, the two atoms are pulled closer together, leading to a decrease in bond length. Thus, for a given pair of atoms, a triple bond is shorter than a double bond, which is shorter than a single bond.

2. Bond Energy

Bond energy is the energy required to separate two bonded atoms. For a given pair of atoms, the strength of a bond (and therefore the bond energy) increases as the number of shared electron pairs increases.

3. Bond Order

Bond order is the number of bonds between two elements in a covalent bond. Bond order is related to bond length and bond energy. Bond order can be determined by several methods (see discussion on bonding theories). In general, as the bond order (number of bonds) increases, the bond energy increases, and the bond length decreases. A single bond has a bond order of 1, double bond a bond order of 2, and a triple bond has a bond order of 3.

Covalent Bond Notation

The shared valence electrons of a covalent bond are called the bonding electrons. The valence electrons not involved in the covalent bond are called nonbonding electrons. The unshared electron pairs can also be called lone electron pairs. A convenient notation, called a Lewis structure is used to represent the bonding and nonbonding electrons in a molecule, facilitating chemical "bookkeeping."

1. Lewis Structures

Write the skeletal structure of a compound (i.e., the arrangement of atoms). For this exercise, you must recall the bonding tendencies of the elements. For example, HCN:

$$\mathrm{H{-}C{-}N} \quad \text{or} \quad \mathrm{H{-}C{\equiv}N}$$

Count all valence electrons of the atoms:
H has 1 valence electron
C has 4 valence electrons
N has 5 valence electrons
10 valence electrons

Obey the octet rule and minimize formal charge while filling in the remaining valence electrons not accounted for in the skeletal structure.

$$\mathrm{H{-}C{\equiv}N{:}}$$

2. Formal charges

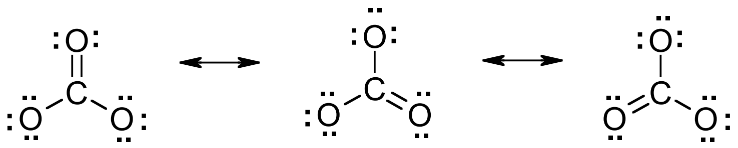
The number of electrons officially assigned to an atom in a Lewis structure does not always equal the number of valence electrons of the free atom. The difference between these two numbers is the formal charge of the atom. Formal charge can be calculated using the following formula:

$$Formal\ charge = valence\ electrons - \frac{1}{2} bonding\ electrons - nonbonding\ electrons$$

The sum of all the formal charges equals the total charge on the molecule or ion. We calculate formal charges on individual atoms by subtracting the number of valence electrons assigned to an atom in its bonded state from the number of valence electrons it has as a neutral free atom.

3. Resonance

For some molecules, two or more Lewis structures are needed to illustrate "snapshots" of the actual molecule. These "snapshots" are called resonance structures. The combination (or weighted average of the structures) of the resonance form more accurately describes the molecule, and is known as the resonance hybrid. Resonance structures are represented with a double- headed arrow between them. It is important to note that the arrows of this type: $\rightleftharpoons$ describes equilibrium, and arrows of this type: $\longleftrightarrow$ describes resonance; a subtle but VERY IMPORTANT difference. See the structure of carbonate below:



All three represent the structure of carbonate. Each Lewis structure represents a resonance form, and all three (since the energies are equivalent) averaged together represent the resonance hybrid. Resonance structures are not structures for the actual molecule or ion; they exist only on paper!

Summary Rules for Resonance:

1. Resonance structures exist only on paper.
2. In writing resonance structures we are only allowed to move electrons.
3. All of the structures must be proper Lewis structures.
4. The energy of the actual molecule is lower than the energy that might be estimated for any contributing structure.
5. Equivalent resonance structures make equal contributions to the hybrid, and a system described by them has a large resonance stabilization.
6. The more stable a structure is (when taken by itself), the greater its contribution to the hybrid. a) The more covalent bonds a structure has, the more stable it is. b) Structures in which all of the atoms have a complete valence shell of electrons (i.e., s^2p^6) are especially stable and make large contributions to the hybrid. c) Charge separation decreases stability. d) Resonance contributors with negative charge on highly electronegative atoms are more stable than ones with negative charge on less or nonelectronegative atoms.

Theories of Chemical Bonding: VB; VSEPR; MO

Many molecules contain atoms bonded according to the octet rule. Exceptions to this rule include, but are not exclusive to: hydrogen (duet), lithium (duet) beryllium (quartet), boron (sextet), and elements below the second period which can have "expanded octets."

1. Valence Shell Electron Pair Repulsion (VSEPR) Theory

The valence shell electron pair repulsion (VSEPR) theory uses Lewis structures to predict the molecular geometry of covalently bonded molecules. It states that the three-dimensional arrangement of atoms surrounding a central atom is determined by the repulsions between the bonding and the nonbonding electron pairs in the valence shell of the central atom. These electron pairs arrange themselves as far apart as possible, thereby minimizing repulsion.

2. Valence Bond (VB) Theory

This theory involves the hybridization of he central metal ion in a transition metal complex. The formation of empty hybrid orbitals on the central metal ion enables a ligand to donate a pair of electrons to form a covalent bond with the ligand positioned in a definite geometry. Geometry, magnetic properties and the possibility of color are predicted.

3. Molecular Orbital (MO) Theory
Theory describes the arrangement of electrons between two nuclei by considering wave functions (ψ) and symmetry restrictions. Predicts bond orders, relative bond energies and magnetic properties.

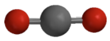
4. Orbital Hybridization
The formation of hybrid atomic orbitals on a central atom accounts for directional bonds. Bond orders, relative bond lengths, polarity (dipole moment) and planarity are predicted. This theory is most applicable to compounds containing carbon or nitrogen.

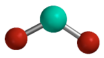
Molecular Geometry (Shape)

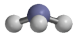
1. Molecular Geometry
Geometry is determined by the number of bonding and unshared pairs of electrons on the central atom. *Shape* indicates that the bonding and nonbonding (unshared) electrons pairs repel each other.

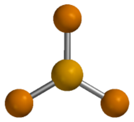
Rules used to predict molecular geometry:

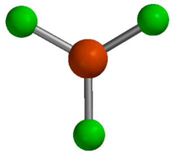
(1)Count the number of valence electrons. (2) Place a pair of electrons between the atoms bound together. (3) Each non-central (terminal) atom is given electrons for its inert gas configuration. (4) Any additional electron pairs become lone (unshared) electrons pairs on the central atom. (5) The geometry is determined by the number of bonding and unshared pairs of electrons on the central atom.
Here are some example structures for molecules and polyatomic ions that consist of a central A atom bonded to two or three B atoms.











	CO_2	SO_2	NH_3	BCl_3	BrF_3
	C-O-C	O-S-O	H-N-H	Cl-B-Cl	F-Br-F
Bond angle	180°	119.3°	106.7°	120°	86.2°
Molecular geometry	Linear	Bent	Trigonal pyramidal	Trigonal planar	T-shaped*

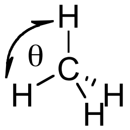
*This term can be very misleading. This structure does not resemble a "T" shape.

Summary of Observed Geometries:

No. of Lone Electron Pairs	Atoms Bound to the Central Atom					
	1	2	3	4	5	6
0	linear	linear	trigonal planar	tetrahedral	trigonal bipyramidal	octahedral
1	linear	bent (120°)	trigonal pyramidal	sawhorse seesaw	square pyramidal	
2	linear	bent (109°)	T-shaped	square planar		
3	linear	linear				

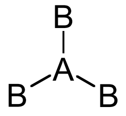
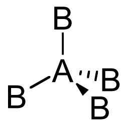
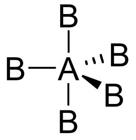
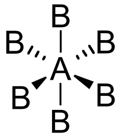
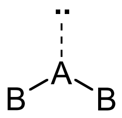
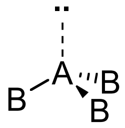
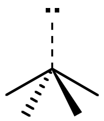
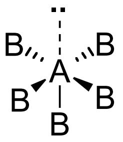
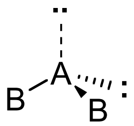
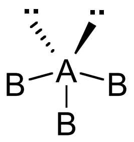
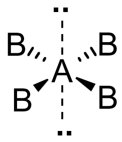
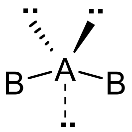
2. Bond Angles

Bond angles are the angles that result from the atomic arrangement, or the geometry of a molecule or ion. The bond angle can be predicted from the VSEPR geometry of a molecule or ion. In a tetrahedral arrangement, for example, the bond angles will be measured as follows:



where $\theta = 120^{\circ}$

Overview of molecular geometries

Electron Pairs	2	3	4	5	6
Molecular Geometry: Zero Lone Pairs	B—A—B Linear	 Trigonal planar	 Tetrahedral	 Trigonal bipyramidal	 Octahedral
Molecular Geometry: One Lone Pair		 Bent (V-shaped)	 Trigonal pyramidal	 Seesaw	 Square pyramidal
Molecular Geometry: Two Lone Pairs			 Bent (V-shaped)	 T-shaped	 Square planar
Molecular Geometry: Three Lone Pairs				 Linear	