CHEMISTRY I

Notes for First Semester College Chemistry

Modern Atomic Theory by John Dalton:

1) All matter is composed of atoms. An Atom is the smallest particle of an element that takes part in chemical reactions.
2) All atoms of a given element are alike, that is, all atoms of gold are the same. Atoms of different elements are different.
3) Compounds are combinations of atoms of more than one element; in a given compound, the relative number of each type of atom is always the same. For example, in water there are always two hydrogen atoms for each oxygen atom.
4) Atoms cannot be created or destroyed. Atoms of one element cannot be changed into atoms of another element by chemical means.

Statement 1 has been revised since atoms can exchange electrons. Statement 2 has been revised due to the existence of isotopes. Statement 3 is still accepted. Statement 4 is true for *chemical* reactions.

Isotopes are atoms of the same element that vary in the number of neutrons.

The nucleus is the small, dense, positively charged center of an atom and contains most of the atom's mass. Electrons account for most of the *size* of an atom. Protons and neutrons are nearly equal in mass. Atoms are electrically neutral.

Atomic Number is the number of *protons*, the whole number on the periodic table, same as the number of electrons in *atoms*.

Mass Number is the sum of protons and neutrons. The hydrogen isotope having a mass number of 2 may be written as H-2 or ${}^{2}_{1}\mathrm{H}$. 1 is the atomic number.

The atomic weight shown on the periodic table is the number of grams in 1 mole of the element; units of g mol.

Gram formula mass has the units g.

A nuclide is an entity, atom, isotope, molecule, etc.

An atomic mass unit is equal to 1/12 of C-12 and is abbreviated as u or amu.

Formula mass is the sum of the atomic masses of a compound.

1 mole is equal to 6.022×10^{23} particles. This value is known as Avogadro's number. It is an approximate value.

Isotopes are atoms of the same element that differ in the number of neutrons.

	Hydrogen Isotopes			Carbon Isotopes		
	H-1	H-2	H-3	C-12	C-13	C-14
Protons	1	1	1	6	6	6
Neutrons	0	1	2	6	7	8
Electrons	1	1	1	6	6	6
Mass #	1	2	3	12	13	14

THE PERIODIC TABLE

Vertical columns are called families or groups.
Horizontal rows are called series or periods.
Alkali metals - group I - very reactive, soft, silvery
Alkaline Earth metals - group IIA -
Halogens - group VIIA
Noble Gases - group 0, virtually non-reactive
Transition elements - in short columns
Inner transition elements - columns listed separately at the bottom
Main group or representative elements - elements other than transitions and inner transitions

MOLECULES result when atoms of (usually) non-metals combine to form compounds or molecular elements. These are covalent bonds and result from electron sharing.

IONIC COMPOUNDS are formed by the transfer of electrons. A positive ion (cation) combines with a negative ion (anion) to form a neutrally charged compound.

Chemistry is the science that deals with the composition, structure, and properties of matter and the changes that matter undergoes.

Matter is anything that occupies space.

In writing a formula, the element furthest to the left on the periodic table is usually written first. If in the same column, the lowest is usually written first. Exceptions are: NH_3 (ammonia), NH_4^+ (ammonium ion), CH_4 (methane).

IONS are formed by the transfer of electrons from one atom to another. Metals have a tendency to lose electrons, becoming positive. Non-metals tend to gain electrons.

Empirical Formula is a chemical formula indicating the variety and relative proportions of the atoms in an ionic compound but not showing the manner in which they are linked together. It is possible to calculate empirical formulas from percent composition. Formula units are ionic compounds.

Molecular Formula is a better representation for a covalent substance because it represents the actual composition. Sometimes empirical and molecular formulas are the same thing. H_2O is an example.

Isomers have the same molecular formula but different connectivities, different properties and characteristics.

The Scientific Method:

1. Observation
2. Formulation of a theory
3. Testing the theory

A coefficient distributes to all subscripts in a formula–not just the ones in parenthesis.

Naming covalent compounds: If a compound is made up of only 2 elements and is not water, then we name it as though it was an ionic compound. If it is 2 non-metals, the 1st is hydrogen. Some binary (means 2 non-metals) covalent compounds can be named using the Greek prefixes (they correspond to the subscripts). If the subscript of the first element is 1, then the first word of the name is the name of that element. i.e. CO_2 is carbon ... If the first subscript is other than 1, then start the first word with a prefix. The second word in the name *always* starts with a prefix as defined by its subscript. The suffix of the second word is *ide*. CO_2 (carbon dioxide), CO (carbon monoxide), N_2O_5 (dinitrogen pentoxide)

The following subscripts that may appear after elements or compounds describe its state:

- (g) - gas
- (l) - liquid
- (s) - solid
- (aq) - aqueous (in water solution)

Hydrogen chloride, HCl, is normally a gas. When in water ($HCl_{(aq)}$) it is hydrochloric acid.

qualitative term: longer (an example)

quantitative term: a number and a unit label

SI Units: International System of Units, derived from the metric system.

derived units are units created from the base units of meter, kilogram, liter, second, ampere, Kelvin, candela, mole.

English System: ounces, pounds, inches, quarts, etc.

Kelvin temperature is denoted with a capital K, not °K.

K = (°C + 273.15)

°F = 9/5 × °C + 32

Bromine is a liquid.

Iodine is a solid.

Precision is the repeatability of a measurement. It also involves significant figures.

Accuracy is how close a measured value is to a known value. It also involves significant figures.

Significant Figures. When multiplying or dividing, round the answer to the number of significant digits in the given value which has the least significant digits. When adding or subtracting, round the answer to the rightmost decimal place precision of the given value which is carried the fewest number of places to the right.

Extensive properties depend on the quantity or amount of substance, for example: mass, volume, length.

Intensive properties are independent of the quantity or amount of substance, for example: density, melting point, boiling point, color, conductivity, whether or not the substance is magnetic.

Density usually decreases with increasing temperature.

density = mass ÷ volume

- solids - g/cm^3
- liquids - g/mL
- gases - g/L

STOICHIOMETRY

Stoichiometry is the study of the quantitative relationships between substances undergoing chemical changes.

Law of Conservation of Matter In chemical reactions, the quantity of matter does not change. Total mass remains the same.

1 mole of oxygen means 1 mole of O_2.

Limiting reactant is the substance in short supply or the substances that will react totally.

Excess reactant is what is left over or does not react in a mixture.

Electrolytes are substances or compounds that conduct electricity when dissolved or melted. The conduction of electricity is due to ions. Putting an ionic compound in solution allows ions to separate from the compound. With a *strong* electrolyte, most of the particles separate into ions in solution. Barium Sulfate $BaSO_4$ is a *strong* electrolyte but is insoluable in water, therefore conductivity is weak even though the electrolyte is considered *strong.* Water and ammonia are *weak* electrolytes. There are 6 acids that are *strong* electrolytes. All other may be considered *weak*.

- $HCl_{(aq)}$ - hydrochloric acid
- $HBr_{(aq)}$ - hydrobromic acid
- $HI_{(aq)}$ - hydriodic acid
- $HClO_{4(aq)}$ - perchloric acid (unstable unless dissolved)
- $HNO_{3(aq)}$ - nitric acid
- $H_2SO_{4(aq)}$ - sulfuric acid

The *hydroxides* of all IA metals and the bottom 4 of the IIA metals are *strong* electrolytes. *Salts* are strong electrolytes. *Metallic hydroxides* may be assumed to be strong electrolytes. Non-electrolytes do not conduct electricity. A reaction between *electrolyte solutions* will take place if either of the possible products is *insoluble* or a *weak* or *nonelectrolyte*.

Acids increase the concentration of *hydrogen ions* when dissolved in water. If the formula starts with H, it might be an acid. If the compound can be broken into H^+ and a common negative ion then it's an acid when combined with water. Acids form ions in water. *Binary acids* are hydrogen plus one element.

Bases are compounds that increase the concentration of hydroxide ions when dissolved in water. Sodium hydroxide NaOH, barium hydroxide $Ba(OH)_2$, and ammonia NH_3 are common *bases*.

Salts are ionic compounds of metals (or polyatomic cations) and nonmetals (or polyatomic anions), except for oxides and hydroxides which are usually classified as *bases*. Salts are formed when aqueous acids react with metallic hydroxide bases.

A single replacement reaction is a reaction between an element and an ionic compound.

In a double replacement reaction two ionic compounds exchange ions.

Ionizable hydrogens are written at the beginning of the formula. $HC_7H_5O_7$

Insoluable means that less than 1/10 gram dissolves in 100 mL of water.

Slightly soluable means that 1/10 gram to less than 1 gram dissolves in 100 mL of water.

Soluable means that 1 gram or more will dissolve in 100 mL water.

A compound that is *insoluble* in water will dissolve in another substance if a weak electrolyte is formed.

In a complete ionic equation, the $_{(aq)}$ is left off and ions are shown separated except where they have formed solids or gases. Ions that appear on both sides of this equation are called spectator ions. In a net ionic equation ions that are free on both sides of the equation are removed. Different *complete ionic equations* could result in the same *net ionic equation*. In a molecular equation, ions are not shown separated.

Very reactive metals react with water to produce a metallic hydroxide and hydrogen gas. These are the metals of group IA and Ca and below in group IIA.

Less reactive metals, if they react with water, will produce metallic oxide and hydrogen gas.

Non-metal *reactivity* decreases down the chart. Metal *reactivity* increases down the chart.

Concentration may be expressed as percent mass or percent volume and should be stated.

There can be *intermingling* and *packing* between molecules so that sometimes the total volume of mixtures will be less than expected: 70 mL alcohol + 30 mL water = 97.4 mL liquid.

Molarity (M) is the number of moles of solute per liter of solution. In calculating dilutions, $M_1 \times V_1 = M_2 \times V_2$, where M is molarity and V is volume.

Titration is a method of determining the amount of substance in a solution by testing with a primary solution. The endpoint of titration is when the amount of the required reactant has been added, which is evidenced by an indicator, such as a change in color of the solution or litmus paper.

A primary standard is a solution of known molarity made from a relatively nonhygroscopic (doesn't tend to absorb water from the atmosphere) solute in pure form (>99.9%).

A standard solution is a solution of known concentration.

Litmus paper: blue paper turns red - acid
red paper turns blue - basic

phenolphthalein: colorless in acid
pink in base
pale pink in a neutral solution

GASES

Vapors are substances which are in the gaseous state that do not normally exist as gases. Mixtures of gases are homegenous. Homogenous mixtures are solutions.

Pressure is force per unit area.

1 atm = 760 torr = 760 mmHg = $1.013\ 25 \times 10^5$ Pa (Pascals) 1 Pa = 1 $kg/m \cdot s^2$

A manometer measures the pressure of a collected gas.

Ideal Gases: The identity of the gas has no effect on its pressure to volume relationship.

Real Gases: Possess the characteristics of ideal gases at high temperatures and low pressures.

Boyle's Law: Pressure is *inversely* proportional to volume, assuming constant temperature.

$$P \times V = k, \text{ a constant}$$

Charles's Law: The volume of a gas is *directly* proportional the Kelvin temperature, assuming constant pressure.

$$V/T = k, \text{ a constant} \qquad V_1/T_1 = V_2/T_2$$

Combined Gas Law:

$$V_2 = V_1 \times P_1/P_2 \times T_2/T_1$$

Gay-Lussac's Law: The volumes of gases involved in chemical reactions are the ratios of small whole numbers, assuming constant temperature and pressure.

$$T_1/P_1 = k \qquad T_1/P_1 = T_2/P_2$$

Avogadro's Law: The volume of a gas is *directly* proportional to the number of molecules.

$$V = k \times n$$

Dalton's Law of Partial Pressures: The total pressure of a mixture of gases is equal to the sum of the partial pressures of the individual gases. Partial pressure of a gas is the pressure that the individual gas exerts in a mixture. One gas pressure does not affect the pressure of another gas in a mixture of gases. When making calculations, assume each gas occupies the entire volume.

Graham's Law: (where MM is molecular mass)

$$\frac{\text{Rate of diffusion of gas 1}}{\text{Rate of diffusion of gas 2}} = \sqrt{\frac{\text{MM gas 2}}{\text{MM gas 1}}}$$

Lighter gases spread out (diffuse) more quickly.

Effusion is the flow of gas through a very small opening.

Ideal Gas Equation: PV = nRT
R = 62.36 when P is expressed in mmHg
R = 0.082 06 when P is expressed in atm
V is in liters, n is moles, T is in Kelvin

Standard Temperature and Pressure (STP): 0°C or 273.15 K and 760 mmHg or 1 atm.

STP molar volume of a gas: 22.4 L (1 mole = 22.4 L)

GASES:
1) Gases consist of very small particles compared to the space occupied. Molecules of Ideal Gases are considered points having no volume.
2) Gas molecules move at high speeds, in thousands of miles per hour.
3) Molecules of Ideal Gases cannot hit each other since they have no volume, but do hit the sides of the container, resulting in pressure on the container.
4) There are no attractive or repulsive forces between Ideal Gas molecules. When one molecule hits another, energy can be transfered but total energy remains unchanged.

5) Kinetic Energy is energy of motion. The average kinetic energy of the molecules is proportional to the Kelvin temperature. avg. kinetic energy = k × T

$$KE = \frac{1}{2}mv^2$$

Density = mass / volume

ENTHALPY

Thermodynamics is the relationship between heat and power.

Thermochemistry is the part of thermodynamics that deals with chemical reactions and heat.

System is the part of the universe a scientist is interested in.

Surroundings is the remainder of the universe.

Universe is the system plus the surroundings.

Exothermic describes a change that produces heat, usually spontaneous.

Endothermic describes a change that cools the surroundings, usually nonspontaneous.

1 calorie = 4.184 Joules (exactly)

Thermal energy is an energy of motion of molecules.

Heat is thermal energy transfer.

Thermal Energy Change [joules] = mass [grams] × specific heat [joules/(gram·°C)] × ΔT [°C]

Heat Capacity = (mass × specific heat) [joules/°C] It is an *extensive* property because it depends on the amount of mass.

Specific Heat is the amount of thermal energy needed to raise 1 gram by 1 °C. [joules/(gram·°C)] It is an *intensive* property because it doesn't depend on the amount of sample.

An exothermic change is indicated by a *negative* sign. Heat is released or lost to the surroundings.

An enthalpy change (ΔH) [kilojoules (kJ)] is a change in thermal energy when a change takes place under constant pressure. In a thermochemical equation, the coefficients stand for the number of *moles*. The reaction: $H_{2(g)} + Cl_{2(g)} \rightarrow 2HCl_{(g)}$ + 184.62 kJ means that the material gets hot, is exothermic. It could also be expressed: $H_{2(g)} + Cl_{2(g)} \rightarrow 2HCl_{(g)}$ ΔH_{rxn} = -184.62 kJ Note the change in sign of the two statements.

Hess's Law The thermal energy transfer in a given change is the same whether it occurs in a single step or several steps.

State Function a property that depends only on the initial and final states of the system. such as enthalpy, pressure. A system is said to be in a certain state when its properties have certain values.

In a formation reaction, one compound is formed from its elements.

In a combustion reaction, a (usually one) substance reacts with oxygen. Usually CO_2 is a/the product. It is always exothermic.

Standard Enthalpy of Formulation $\Delta H°_f$ [kJ/mol] is the amount of energy involved when one mole of the substance is formed @ 25 °C. The standard form of an element has a standard enthalpy of formation of 0 kJ/mol. The standard enthalpy of a reaction $\Delta H°_{rxn}$ is equal to the sum of the product enthalpies minus the sum of the reactant enthalpies. Remember that the standard enthalpy of an element in its standard form is zero.

ATOMIC THEORY

The Heisenberg Uncertainty Principle helps to describe the locations of electrons in terms of probability. It indicates that we cannot describe the exact location of an electron.

The quantum mechanical or the wave mechanical model of the atom is a theory for the description of the makeup of the atom. It is highly Calculus based and is based on the Schrödinger Equation.

An orbital is the volume in space where an electron of particular energy is likely to be found. An electron in one orgital will have a different energy than an electron in another orbital.

Electron energies are said to be quantized, that is, they have different sets of energies. If an electron loses or gains energy, it will do so only in regular or set quantities. When all of the electrons in an atom are in their lowest possible levels or positions, the atom is said to be in the ground state. When one or more of the electrons are in higher energy levels, the atom is said to be in the excited state.

The first shell, which is indicated by n=1, contains one s sublevel. The s sublevel is spherical in shape and is indicated by $l=0$ (that's an el).

The second shell, which is indicated by n=2, contains an s and a p sublevel. There are three orbitals in a p sublevel. They are shaped like ∞. $l=1$ indicates a p sublevel.

The third shell, which is indicated by n=3, contains an s sublevel, a p sublevel, and a d sublevel. A d sublevel is indicated by $l=2$ and contains 5 orbitals. Don't worry about the shapes of these orbitals.

This pattern of shell construction continues with an f sublevel, indicated by $l=3$, containing 7 orbitals, a g sublevel, indicated by $l=4$, containing 9 orbitals, and an h sublevel, indicated by $l=5$, containing 11 orbitals.

A particular orbital is indicated by its magnetic quantum number, m_l. The value of m_l may be from $-l$ to $+l$. An orbital may have zero, one, or two electrons. The particular electron is indicated by a spin quantum number, m_s, which may be equal to -½ or +½.

By the Aufbau Principle, electrons are put into lowest orbitals first.

By Hund's Rule, when electrons are put into orbitals having the same energy (degenerate orbitals), one electron is put into each orbital before putting a second electron into an orbital. For example, a given p sublevel contains 3 *degenerate* orbitals. One electron will be placed in each of these orbitals before a second electron is placed in any of them.

Atoms with unpaired electrons are <u>paramagnetic</u>. Paramagnetic materials are weakly magnetized when brought into proximity to a magnet.

Atoms with no unpaired electrons are <u>diamagnetic</u>.

An <u>octet</u> has all orbitals in the first two shells filled.

By the <u>Pauli Exclusion Principal</u>, no 2 electrons in a given atom can have all 4 quantum numbers alike.

<u>Orbital Notation</u> example:

$$\underset{1s}{\uparrow\downarrow}\ \underset{2s}{\uparrow\downarrow}\ \underset{2p}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}\ \underset{3s}{\uparrow\downarrow}\ \underset{3p}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}\ \underset{4s}{\uparrow\downarrow}\ \underset{3d}{\uparrow\ \uparrow}$$

$$\underset{1s}{\boxed{\uparrow\downarrow}}\ \underset{2s}{\boxed{\uparrow\downarrow}}\ \underset{2p}{\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}}\ \underset{3s}{\boxed{\uparrow\downarrow}}\ \underset{3p}{\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}}\ \underset{4s}{\boxed{\uparrow\downarrow}}\ \underset{3d}{\boxed{\uparrow}\boxed{\uparrow}}$$

<u>Electron Configuration Notation</u> example; note the order by shell number:

Ti Titanium $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^2\ 4s^2$

<u>Abbreviated Orbital Notation</u> example; the symbol for the noble gas preceeding the element is written in brackets (this is called the <u>core</u>), then additional electrons are shown following:

Ti Titanium [Ar] $\underset{4s}{\uparrow\downarrow}\ \underset{3d}{\uparrow\ \uparrow}$

<u>Abbreviated Electron Configuration Notation</u> example:

Ti Titanium [Ar] $3d^2\ 4s^2$

<u>Ionization energies</u> generally decrease to the lower left. This is because those elements tend to have more shells so that the outer electrons are less tightly held.

When an atom loses electrons this happens in the reverse order of <u>electron configuration notation</u>. Outermost electrons leave the atom first, even though a lower shell might not be filled. In the case of our Titanium example, electrons would leave the 4s shell first although the 3d shell is not filled. <u>Returning electrons</u> fill the previously vacated spots first, then additional filling is according to Hund's Rule.

<u>Exceptions to Hund's Rule</u>:

Cr	[Ar] $3d^5\ 4s^1$
Mo	[Kr] $4d^5\ 5s^1$
Cu	[Ar] $3d^{10}\ 4s^1$
Ag	[Kr] $4d^{10}\ 5s^1$
Au	[Xe] $4f^{14}\ 5d^{10}\ 6s^1$
Pd	[Kr] $4d^{10}$
Pt	[Xe] $4f^{14}\ 5d^9\ 6s^1$

<u>Valence Electrons</u> are the electrons in the outer **shell**.

<u>first ionization energy</u>: The amount of energy needed to remove one electron each from one mole of gaseous atoms. In general, the highest first ionization energies belong to atoms in the upper right corner of the periodic chart. Endothermic.

<u>second ionization energy</u>: Stronger than first ionization energy.

<u>electron affinity</u>: The measure of an atom's tendency to gain an electron. Thermal energy is released from most atoms when they gain an electron. Exothermic. The higher the electron affinity number, the more likely to gain an electron.

<u>atomic radii</u>: *Main* group radii generally increase to the lower left. Two factors influence the size of the radii:

1) The attraction of the positively charged nucleus to the negatively charged electrons
2) The negatively charged electrons tend to repel each other.

Additional shells tend to resist the effect of 1) due to <u>electron shielding</u>. The pull of the nucleus on the outer electrons is partially blocked by the inner electrons.

<u>Lanthanide Contraction</u>: Groups of transition elements tend to be about the same size.

<u>Isoelectronic</u>: having the same electron configuration, such as:

$\mathbf{Na^{1+}}$	$1s^2\ 2s^2\ 2p^6$
$\mathbf{F^{1-}}$	$1s^2\ 2s^2\ 2p^6$
Ne	$1s^2\ 2s^2\ 2p^6$
$\mathbf{O^{2-}}$	$1s^2\ 2s^2\ 2p^6$
$\mathbf{Mg^{2+}}$	$1s^2\ 2s^2\ 2p^6$
$\mathbf{Al^{3+}}$	$1s^2\ 2s^2\ 2p^6$

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