REVIEW: TOPIC 3
MOLES + STOICHIOMETRY

Name: ____________

Due: ____________

UNIT 3 – MAJOR UNDERSTANDINGS

- ☆ 3.1cc A compound is a substance composed of two or more different elements that are chemically combined in a fixed proportion. A chemical compound can be broken down by chemical means. A chemical compound can be represented by a specific chemical formula and assigned a name based on the IUPAC system.
- ☆ 3.1ee Types of chemical formulas include empirical, molecular, and structural.
- ☆ 3.3d The empirical formula of a compound is the simplest whole-number ratio of atoms of the elements in a compound. It may be different from the molecular formula, which is the actual ratio of atoms in a molecule of that compound.
- ☆ 3.3a In all chemical reactions there is a conservation of mass, energy, and charge.
- ☆ 3.3c A balanced chemical equation represents conservation of atoms. The coefficients in a balanced

UNIT 3 – MAJOR UNDERSTANDINGS (CONTINUED)

chemical equation can be used to determine mole ratios in the reaction.

- ☆ 3.3e The formula mass of a substance is the sum of the atomic masses of its atoms. The molar mass (gram-formula mass) of a substance equals one mole of that substance.
- ☆ 3.3f The percent composition by mass of each element in a compound can be calculated mathematically.
- ☆ 3.2b Types of chemical reactions include synthesis, decomposition, single replacement, and double replacement.

A **compound** is a substance composed of two or more different elements that are chemically combined in a fixed proportion and can be broken down by chemical means. Chemical compounds are represented by a specific formula and assigned a name based on the IUPAC system. Examples are H_2O (water = dihydrogen oxide), CO_2 (carbon dioxide), CCl_4 (carbon tetrachloride).

A – FORMULA WRITING

A **symbol** may represent one atom or one mole of atoms of an element. One mole of atoms contains Avogadro's number (6.02×10^{23}) of atoms. A **formula** is a statement in chemical symbols that represents the composition of a substance.

CHEMICAL FORMULA

A **chemical formula** is both a qualitative and a quantitative expression of the composition of an element or a compound. For example, the formula for phosphoric acid is H_3PO_4. This formula describes a molecule of phosphoric acid composed of 3 atoms of hydrogen, 1 atom of phosphorus, and 4 atoms of oxygen. It also states that to make a mole of this compound, 3 moles of hydrogen atoms, 1 mole of phosphorus atoms, and 4 moles of oxygen atoms are needed.

There are three basic types of formulas:

- An **empirical formula** represents the simplest whole number ratio in which elements combine to form a compound. For example, the empirical formula for H_2O_2 is HO.

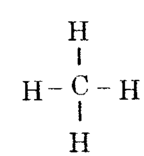
- The **molecular formula** is the whole number multiple of the empirical formula, and indicates the total number of atoms of each element needed to form the molecule, given the mole mass of substance. The formula mass of the empirical formula CH is 12 + 1 = 13. The molecule with the same empirical formula but with a mass of 78 is C_6H_6.

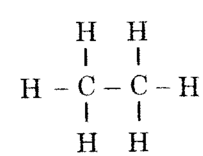
  Given the empirical formula and the molecular mass, it is possible to derive the molecular formula:

  1) determine the formula mass of the empirical formula,
  2) divide this formula mass into the molecular mass, and
  3) multiply this result by the subscript of each atom in the compound.

- The **structural formula** demonstrates the connections between atoms of a molecule or ion in space.

Examples include: **CH_4** **C_2H_6**





B – Naming & Writing Chemical Compound Formulas

The common oxidation number (state) is found in the *Periodic Table of Elements* and is given for each of the elements. It represents the charge which an atom has, or appears to have, when the electrons are counted according to certain arbitrary rules. These rules result in the following operational rules for determining oxidation numbers.

- In the free element, each atom has an oxidation number of zero.
- In simple ions (ions containing one atom), the oxidation number is equal to the charge on the ion.
- The algebraic sum of all the oxidation numbers of the atoms of any molecule or compound is zero.
- The oxidation number of oxygen is -2, except in peroxides it is -1.
- Oxidation number of hydrogen is +1, except in hydrides it is -1.
- In nonmetal compounds, the less electronegative element is positive; the more electronegative element is negative.
- The algebraic sum of the charges of the atoms in a polyatomic ion is equal to the charge on the ion.

The chemical name of a compound generally indicates the chemical composition of the substance. The procedure used in naming and writing chemical formulas are as follows.

- In binary compounds composed of metals and nonmetals, the metallic element is usually named and written first. The name of the nonmetal ends in "**–ide**" (for example, sodium chloride, potassium bromide, lithium iodide).
- In compounds composed of two nonmetals, the less electronegative element is usually named and written first. The name of the compound still ends in "–ide" (for example, hydrogen chloride, nitrogen bromide).
- Prefixes are used to indicate the number of atoms of each nonmetal in the compound. Examples include carbon <u>di</u>oxide (CO_2), sulfur <u>tri</u>oxide (SO_3), carbon <u>tetra</u>chloride (CCl_4).
- In the naming of compounds, which include one or more polyatomic ions, the metal is usually named first with polyatomic ions named last (for example, sodium hydroxide – NaOH, magnesium sulfate – $MgSO_4$).

The various **polyatomic ions** and their charges are listed in *Reference Table E.*

In naming compounds of metals which may have more than one oxidation number, the **Stock System** should be used. In this system, Roman numerals indicate the oxidation number of the metal ion. For example, FeO is named iron (II) oxide, and Fe_2O_3 is named iron (III) oxide.

- When a metal is combined with a polyatomic ion, the name of the metal is followed with the name of the polyatomic ion. (Such as Na_2CO_3 – sodium carbonate and $K_2Cr_2O_7$ – potassium dichromate.)

Table E
Selected Polyatomic Ions

H_3O^+	hydronium	CrO_4^{2-}	chromate
Hg_2^{2+}	dimercury (I)	$Cr_2O_7^{2-}$	dichromate
NH_4^+	ammonium	MnO_4^-	permanganate
$C_2H_3O_2^-$ / CH_3COO^-	acetate	NO_2^-	nitrite
		NO_3^-	nitrate
CN^-	cyanide	O_2^{2-}	peroxide
CO_3^{2-}	carbonate	OH^-	hydroxide
HCO_3^-	hydrogen carbonate	PO_4^{3-}	phosphate
$C_2O_4^{2-}$	oxalate	SCN^-	thiocyanate
ClO^-	hypochlorite	SO_3^{2-}	sulfite
ClO_2^-	chlorite	SO_4^{2-}	sulfate
ClO_3^-	chlorate	HSO_4^-	hydrogen sulfate
ClO_4^-	perchlorate	$S_2O_3^{2-}$	thiosulfate

Table E Selected Polyatomic Ions

The polyatomic ions and their names in this table are used when writing formulas and naming compounds. Polyatomic ions bond with metals or other polyatomic ions by means of an ionic bond.

C – Chemical Equations

A chemical equation represents the type and the amount of changes in **bonding** and energy that take place in a chemical reaction. It is made up of **reactants** (those items that enter into the reaction and are usually found on the left side of the equation) and the **products** (those items produced and usually found on the right side of the equation). For example:

$$2H_2 + O_2 \rightarrow 2H_2O + \text{heat}$$

The addition of two molecules of hydrogen and one molecule of oxygen results in the production of two molecules of water and heat. Two moles of hydrogen plus one mole of oxygen results in 2 moles of water molecules. In all reactions there is a conservation of mass, energy, and change.

In an equation, it is often desirable to indicate the phase of reactants and products. This may be done by using the symbols: (***s***) = solid; (***l***) = liquid; (***g***) = gas; and (***aq***) = in an **aqueous solution**. The "written equation" is shown as:

$$2H_2\,(g) + O_2\,(g) \rightarrow 2H_2O\,(l) + \text{heat}$$

Balancing Equations

The number of atoms of each element must be the same on both sides of the equation. This is done by placing numbers in front of the formulas (**coefficients**) in order to equalize the number of atoms.

1) Balancing equations by inspection:

$$\_\_\_\_ H_2(g) + \_\_\_\_ N_2\,(g) \rightarrow \_\_\_\_ NH_3\,(g)$$

In order to balance the number of hydrogen atoms, the common multiple of 2 and 3 which is 6 is used. The coefficient 3 is placed in front of the H_2 on the left side of the equation and 2 in front of the product on the right side:

$$3H_2(g) + N_2\,(g) \rightarrow 2NH_3\,(g)$$

By coincidence, when the hydrogen atoms are balanced, nitrogen atoms are balanced out and the total equation is balanced.

2) Balancing equations with missing valid formulas. The word equation for the reaction of aluminum and sulfuric acid is

Note: Aluminum reacts with sulfuric acid to produce aluminum sulfate and hydrogen gas.

The *Periodic Table* provides the oxidation states which are used to write valid formulas. By writing the individual oxidation state above each atom or polyatomic ion and multiplying it by the number of atoms or polyatomic ions in the formula, the total oxidation state for each is obtained. When the oxidation states for each formula add up to 0, the formulas in the equation are valid.

$$\begin{array}{ccccccccl}
0 & & +2\ +6\ -8 & & +6\quad -6 & & 0 & = 0 & \text{(total oxidation state)} \\
0 & & +1\ +6\ -2 & & +3\quad -2 & & 0 & & \text{(individual oxidation states)} \\
Al(s) & + & H_2SO_4(aq) & \rightarrow & Al_2(SO_4)_3(aq) & + & H_2(g) & &
\end{array}$$

In order to balance the equation the coefficients are added:

$$2Al(s) + 3H_2SO_4(aq) \rightarrow Al_2(SO_4)_3(aq) + 3H_2(g) \quad \text{(balanced equation)}$$

D – Mole Interpretation

A mole contains Avogadro's number (6.02×10^{23}) of particles and may be used in calculations involving the number of particles (atoms, molecules, ions, electrons, or other particles) involved in chemical reactions, the mass of elements or compounds, or the volume relationships in gases.

Gram Atomic Mass (Gram-Atom)

The gram atomic mass (gram-atom) of an element represents the mass in grams of Avogadro's number (6.02×10^{23}) of atoms of the element. The gram-atomic mass is numerically equal to the atomic mass as shown in the *Periodic Table*. For example, the atomic mass of the element sulfur is 32.06 amu. A mole of this element weighs 32.06 grams.

Gram Formula Mass (Molar-Mass)

The gram molecular mass (mass of 1 mole) is the sum of the gram atomic masses of the atoms that make up a particular molecule. The gram formula mass is the sum of the gram atomic masses of the atoms that make up a particular formula. The gram formula mass calculated from the empirical formula is used for ionic substances and network solids, since they are not molecular substances.

Sample Problem: What is the gram molecular mass of water (H_2O)?

Solution:

The gram atomic mass of 1 mole of hydrogen atoms is $1\ g \times 2 = 2\ g$

The gram atomic mass of 1 mole of oxygen atoms is $16\ g \times 1 = 16\ g$

The gram molar mass of water is therefore $16 + 2 = 18$ g/mole

Molar Volume of a Gas

A mole (6.02×10^{23}) of molecules of any gas occupies 22.4 liters at STP. It has a mass equal to the molecular mass expressed in grams.

Problems Involving Formulas

Percent composition – The percent composition by mass of an element in a compound can be calculated by dividing the total mass of that element in the formula by the total **formula mass** of the compound.

Sample Problem: Calculate the percent composition by mass of H_2O.

First, calculate the formula mass by the following method.

Each hydrogen atom has a mass of ... 1 amu = 1 amu × 2 = 2 amu

An oxygen atom has a mass of ... 16 amu = 16 amu × 1 = 16 amu

Total formula mass ... = 18 amu

Second, divide the total mass of each element by the formula mass, and multiply the resulting decimal by 100%.

$$\textbf{hydrogen} = \frac{\textbf{2 amu}}{\textbf{18 amu}} = \textbf{0.11 x 100\% = 11\%} \text{ (answer)}$$

$$\textbf{oxygen} = \frac{\textbf{16 amu}}{\textbf{18 amu}} = \textbf{0.89 x 100\% = 89\%} \text{ (answer)}$$

As noted in *Reference Table T*:

$$\textbf{\% composition by mass} = \frac{\textbf{mass of part}}{\textbf{mass of whole}} \textbf{ x 100\%}$$

Sample Problem: Calculate the percent, by mass, of water of hydration in gypsum ($CaSO_4 \bullet 2H_2O$).

First, calculate the formula mass:

Ca	= 40	x	1	= 40. amu
S	= 32	x	1	= 32. amu
O	= 16	x	6	= 96. amu
H	= 1	x	4	= 04. amu
				172. amu

Second, calculate the mass of water in the compound. As stated above, each water molecule has a mass of 18 amu. Since there are two (2) molecules in the formula, the mass of the water molecules is 36 amu. Divide the mass of the water molecules by the formula mass of the compound and multiple the decimal by 100%.

$$\frac{\textbf{36 amu}}{\textbf{172 amu}} = \textbf{0.21 x 100\% =21\%} \text{ (answer)}$$

Problem: Determine the empirical formula from percent composition.

Step 1 – Divide the percent by the atomic weight.
Step 2 – Divide the result by the lowest number.
Step 3 – Change to the simplest whole number ratio and write formula.

Example: Find and write the empirical formula for 32..8% chromium and 67.2% chlorine.

Step 1 – $\frac{32.8}{52} = 0.63$ mole and $\frac{67.2}{35.5} = 1.89$ moles

Step 2 – $\frac{.63 \text{ mole}}{.63 \text{ mole}} = 1$ (formula units) and $\frac{1.89 \text{ moles}}{.63 \text{ mole}} = 3$ (formula units)

Step 3 – Result: $CrCl_3$

The general types of chemical reactions include the following:

Composition or Synthesis – Two or more substances combine to form a compound.

$$\mathbf{X + Y \rightarrow XY}$$

An example would be:

$$\mathbf{Mg + S \rightarrow MgS}$$
Magnesium + Sulfur → Magnesium Sulfide

Decomposition or Analysis – The opposite of composition:

$$\mathbf{XY \rightarrow X + Y}$$
Magnesium Sulfide → Magnesium + Sulfur

Single Replacement – The displacement of one substance in a compound by another substance:

$$\mathbf{X + YZ \rightarrow XZ + Y}$$
or
$$\mathbf{A + YZ \rightarrow YA + Z}$$

Examples:

$$\mathbf{K + NaCl \rightarrow KCl + Na}$$
$$\mathbf{Cl_2 + 2NaI \rightarrow 2NaCl + I_2}$$

Double Replacement or Ionic Reactions – In this reaction two compounds exchange in the following manner:

$$\mathbf{AB + CD \rightarrow AD + CB}$$

In this reaction a product leaves the solution in the form of a precipitate or gas. One classic example is:

$$NaCl(aq) + AgNO_3(aq) \rightarrow NaNO_3 + AgCl(s)\downarrow \text{ (white precipitate)}$$

Unit Three – Moles & Stoichiometry

Key Concepts

- Compound
- Empirical Formula
- Molecular Formula
- Structural Formula
- Conservation of Mass, Energy, and Charge
- Balanced Equations
- Formula Mass
- Molar Mass (gram-formula mass)
- Percent Composition by Mass
- Types of Chemical Reactions

I. Compounds

A **compound** is a substance composed of two or more different elements that are chemically combined in a fixed ratio (proportion). For example, in calcium chloride ($CaCl_2$) the ratio of calcium to chlorine is 1:2. A chemical compound can be broken down by chemical means. Therefore, calcium chloride can be broken apart into its individual elements . . .

$$CaCl_{2(s)} \rightarrow Ca_{(5)} \rightarrow Cl_{2(g)}$$

There are many ways a compound can be represented. The **empirical formula** of a compound is the simplest whole-number ration of atoms of the elements is a compound. It may be different from the **molecular formula**, which is the actual ratio of atoms in a molecule of that compound.

IUPAC Name	Molecular Formula	Empirical Formula	Structural Formula

Ethene	C_2H_4	CH_2	H — C = C — H
			        | |
			       H H

II. Naming Compounds

a. Ionic Compounds

For ionic compounds the cation (the + ion) always proceeds the anion (the – ion).

$CaCl_2$	Na_2SO_4	$Al(OH)_3$
Calcium Chloride	Sodium Sulfate	Aluminum Hydroxide

b. Molecular (covalent) Compounds

Prefixes like mono, di, tri, tetra, pent, and hex must be used to indicate the number of each element in the compound. The mono is dropped if it is the first element in the compound.

CO	CO_2	N_2O_5
Carbon Monoxide	Carbon Dioxide	Dinitrogen Pentoxide

III. Writing Formulas

a. Ionic Compounds

For ionic compounds the cation (the + ion) and the anion (the - ion) must have their charges balanced when writing the compound.

Barium Flouride	Aluminum Sulfate
Ba^{+2} F^{-1}	Al^{+3} SO_4^{-2}
BaF_2	$Al_2(SO_4)_3$

b. Molecular (covalent) Compounds

For molecular compounds, all you need to do is make sure the number of each element in the compound matches the prefix in the name. Remember if no prefix is on the first word of the compound then there is only one of that element.

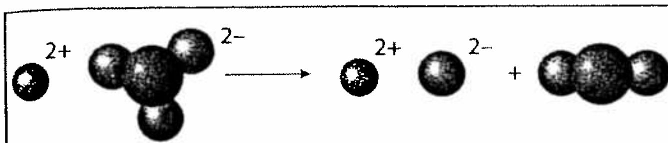
Carbon Dioxide	Dinitrogen monoxide
CO_2	N_2O

IV. Chemical Reaction

In all chemical reactions there is a conservation of mass, energy, and charge. There are 4 types of chemical reactions, synthesis (direct combination) decomposition single replacement, and double replacement.

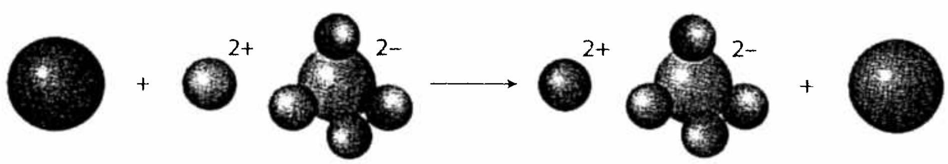
$C(s)$	+	$O_2(g)$	$\longrightarrow$	$CO_2(g)$
A	+	B	$\longrightarrow$	AB

Figure 2-6. Equation of a synthesis reaction: In this example, two elements combine to form a compound.



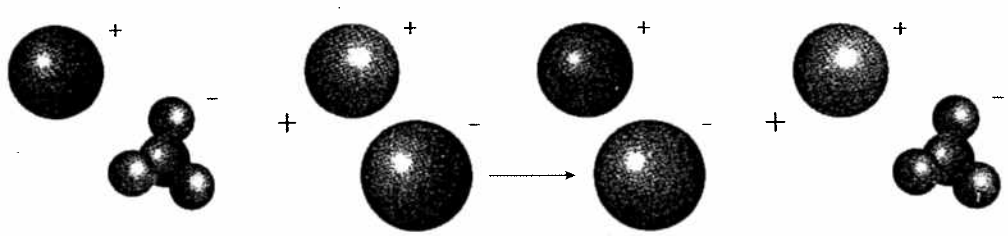
$CaCO_3$	$\longrightarrow$	CaO	+	CO_2
AB	$\longrightarrow$	A	+	B

Figure 2-7. Equation of a decomposition reaction: The models for $CaCO_3$ and CaO show that the compounds are ionic and do not form molecules. They are compounds that exist as ions.



Fe	+	$CuSO_4\,(aq)$	$\longrightarrow$	$FeSO_4\,(aq)$	+	Cu
A	+	BX	$\longrightarrow$	AX	+	B

Figure 2-8. Equation of a single replacement reaction: The copper and iron ions are part of the compounds that are in solution, but the iron and copper atoms are solid metals.

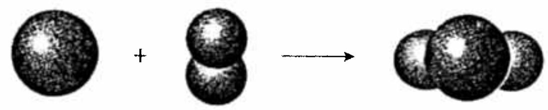


$AgNO_3(aq)$	+	$KCl(aq)$	$\longrightarrow$	$AgCl(s)$	+	$KNO_3(aq)$
AB	+	CD	$\longrightarrow$	AD	+	CB

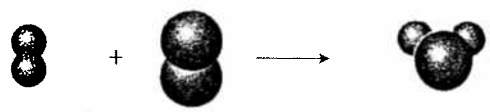
Figure 2-9. An equation for a double replacement reaction: Although all the compounds are ionic, AgCl is an ionic compound that is not soluble in water. Crystals of AgCl form a precipitate.

V. Balancing Chemical Reactions

A balanced chemical equation represents conservation of atoms. The coefficients in a balanced chemical equation can be used to determine mole ratios in the reaction. **Molecular models** can also be used to show a balanced reaction.



Balanced chemical equation:	$C + O_2$ One carbon atom, two oxygen atoms	$\longrightarrow$	CO_2 One carbon atom, two oxygen atoms



Unbalanced chemical equation:	$H_2 + O_2$ Two hydrogen atoms, two oxygen atoms	$\longrightarrow$	H_2O Two hydrogen atoms, one oxygen atom

VI. Stoiciometry

The coefficients in a balanced chemical equation, represent the number of moles of each substance involved in the reaction. The ratio is used to determine an unknown number of moles.

Example Problem: Given 5 moles of nitrogen, calculate the moles of ammonia using the following balanced equation: $N_2 + 3H_2 \rightarrow 2NH_3$

Solution: Ratio of N_2 to NH_3 is 1:2. Since you have 5 moles of N_2 you have 10 moles of NH_3.

VII. More Math Stuff

The **formula mass** of a substance is the sum of the atomic masses of its atoms. The **molar mass (gram-formula mass)** of a substance equals one mole of that substance.

	Formula Mass	Molar Mass
NH_3	14 + 3(1) = 17 AMU	17 grams

The percent composition by mass of each element in a compound can be calculated mathematically.

NH_3 % Nitrogen = 14/17 x 100 = 82.4%

% Hydrogen = 3/17 x 100 = 17.6%

VII. Mole Calculations (see equation on Table T)

Example Problem: Given 2.5 moles of H_2O calculate the number of grams.

Solution: Gram formula mass of H_2O is $2(1) + 16 = 18$ g/mol

$$2.5 \text{ moles} = \frac{\text{X grams of } H_2O}{18 \text{ g/mol}} \qquad X = 45 \text{ grams of } H_2O$$

Example Problem: Given 116 grams of NaCl calculate the number of moles.

Solution: Gram Formula Mass of NaCl is $23 + 35 = 58$ g/mol

$$\text{X moles} = \frac{116 \text{ grams of NaCl}}{58 \text{ g/mol}} \qquad X = 2 \text{ moles of NaCl}$$