# Calculations with Chemical Formulas & Equations(Stoichiometry)

Formula Weight

Formula and Molecular Weights

• **Formula weight** (FW) is the sum of atomic weights for the atoms shown in the *empirical* formula.

• Formula weight of the repeating unit (*formula unit)* is used for ionic substances.

• Example: FW (NaCl) = 22.99 amu + 35.45 amu = 58.44 amu.

• **Molecular weight** (MW) sum of the atomic weights of atoms in a molecule as shown in the *molecular* formula.

• Example: MW (C6H12O6) = 6(12.01 amu) + 12 (1.00 amu) + 6 (16.00 amu) = 180.06 amu.

Percentage Composition from Formulas

• *Percentage composition* is obtained by dividing the mass contributed by each element (number of atoms times AW) by the formula weight of the compound and multiplying by 100.

• Find the % of “C” in C6H12O6

**Avogadro’s Number and The Mole**

• The **mole** (abbreviated "mol") is a convenient measure of chemical quantities.

• 1 mole of something = 6.0221421 x 1023 of that thing. (in most cases 6.02 x 1023 has sufficient sfs)

• This number is called **Avogadro’s number**. Thus, 1 mole of carbon atoms = 6.0221421 x 1023 carbon atoms.

• A mole of marbles would cover the entire surface of the earth to a depth of 3 miles!

Molar Mass

• The mass in grams of 1 mole of substance is said to be the **molar mass** of that substance. Molar mass has units of g/mol (also written g•mol–1).

• By definition, 1 mole of 12C has a mass of exactly 12 g.

• The molar mass of a molecule is the sum of the molar masses of the atoms:

• Example: The molar mass of N2 = 2 x (molar mass of N) = 2 x 14.01g/mole.

• Molar masses for elements are found on the periodic table.

• The formula weight (in amu) is *numerically* equal to the molar mass (in g/mol).

Interconverting Masses and Moles

• To convert between grams and moles, we use the molar mass.

Interconverting Masses and Number of Particles

• Number of particles: 6.022 x 1023/ mol (Avogadro’s number).

• Note: g/mol x mol = g (molar mass x moles = mass)

• # of mols x 6.022 x 1023/ mol = # atoms or molecules, etc

• To convert between moles and molecules we use Avogadro’s number.

Empirical Formulas from Analyses

• Finding empirical formula from mass percent data:

• Given the mass percent of elements, assume a 100 g of sample to calculate mole ratios.

73.90%Hg 73.90g Hg x 1mol/200.59g Hg = 0.36841 mol Hg / 0.36841 = 1

26.10%Cl 26.10g Cl x 1mol/35.45g Cl = 0.73625 mol Cl / = 0.36841 = 1.998 ≈ 2 HgCl2

Molecular Formula from Empirical Formula

• The empirical formula (relative ratio of elements in the molecule) may not be the molecular formula (actual ratio of elements in the molecule).

• Example: ascorbic acid (vitamin C) has the empirical formula C3H4O3 which has a formula weight of 88.07g/mol and a molecular weight of 176.14g/mol.

• The ratio of molecular weight (MW) to formula weight (FW) of the empirical formula must be a whole number.

MW/FW = 176.14/88.07 = 2 therefore the molecular formula is C6H8O6.

Combustion Analysis

• Empirical formulas are routinely determined by combustion analysis.

• A sample containing C, H, and O is combusted in excess oxygen to produce CO2 and H2O.

• The amount of CO2 gives the amount of C originally present in the sample.

• The amount of H2O gives the amount of H originally present in the sample.

• Watch the stoichiometry: 1 mol H2O contains 2 mol H.

• The amount of O originally present in the sample is given by the difference between the amount of sample and the amount of C and H accounted for. See pgs 117-119 Examples 3.20 and 3.21.

# Chemical Equations

• The quantitative nature of chemical formulas and reactions is called **stoichiometry**.

**•** Lavoisier observed that mass is conserved in a chemical reaction: **law of conservation of mass**.

• **Chemical equations** give a description of a chemical reaction .

**reactants** ( left of the arrow) and **products** ( right of the arrow): 2H2 + O2 → 2H2O

• There are two sets of numbers in a chemical equation:

• numbers in front of the chemical formulas (called stoichiometric ***coefficients***) and

• numbers in the formulas (***subscripts***).

• Stoichiometric coefficients give the *ratio* in which the reactants and products exist.

• The subscripts give the ratio in which the atoms are found in the molecule.

• H**2**O means there are two H atoms for each one molecule of water.

• **2**H2O means that there are two water molecules present.

• Note: in 2H2O there are *four* hydrogen atoms present (two for each water molecule).

Balancing Equations

• Matter cannot be lost in any chemical reaction. Therefore, the products of a chemical reaction have to account for all the atoms present in the reactants--we must *balance* the chemical equation.

• When balancing a chemical equation we adjust the stoichiometric coefficients in front of chemical formulas.

• Subscripts in a formula are ***never*** changed when balancing an equation.

• Example: the reaction of methane with oxygen: CH4 + O2 → CO2 + H2O

• Counting *atoms* in the reactants yields: 1 C; 4 H; and 2 O.

• In the products we see: 1 C; 2 H; and 3 O.

• It appears as though an H has been lost and an O has been created.

• To balance the equation, we adjust the stoichiometric coefficients: CH4 + **2**O2 → CO2 + **2**H2O

Indicating the States of Reactants and Products

• The physical state of reactants and products may be added to the equation: CH4(*g*) + 2O2(*g*) → CO2(*g*) + 2H2O(*g*)

• Reaction conditions occasionally appear above or below the reaction arrow

(e.g., "Δ" is often used to indicate the addition of heat, e- means electricity, etc)

Some Simple Patterns of Chemical Reactivity

Combination and Decomposition Reactions

• In **combination reactions** two or more substances react to form one product.

• Combination reactions have more reactants than products.

• Consider the reaction: 2Mg(*s*) + O2(*g*) → 2MgO(*s*)

• Since there are fewer products than reactants, the Mg has combined with O2 to form MgO.

• Note that the structure/properties of the reactants has changed in the product .

• Mg consists of closely packed atoms and O2 consists of dispersed molecules.

• MgO consists of a crystal lattice of Mg2+ and O2– ions (a new substance formed)

• In **decomposition reactions** one substance undergoes a reaction to produce two or more other substances.

• Decomposition reactions have more products than reactants.

• Consider the reaction that occurs in an automobile air bag: 2NaN3(*s*) —Δ→ 2Na(*s*) + 3N2(*g*)

• Since there are more products than reactants, the sodium azide has decomposed into sodium metal and nitrogen gas.

Combustion in Air

• **Combustion reactions** are rapid reactions that produce a flame.

• Most combustion reactions involve the reaction of O2(*g*) from air.

• Example: combustion of a hydrocarbon (propane) to produce carbon dioxide and water.

C3H8(*g*) + 5O2(*g*) → 3CO2(*g*) + 4H2O(*l*)

Quantitative Information from Balanced Equations

• The coefficients in a balanced chemical equation give the relative numbers of molecules (or formula units) involved in the reaction.

• The stoichiometric coefficients in the balanced equation may be interpreted as:

• the relative numbers of molecules or formula units involved in the reaction or

• the relative numbers of moles involved in the reaction.

• The molar quantities indicated by the coefficients in a balanced equation are called *stoichiometrically equivalent quantities*.

• Stoichiometric relations or ratios may be used to convert between quantities of reactants and products in a reaction.

• It is important to realize that the stoichiometric ratios are the ideal proportions in which reactants are needed to form products.

• The number of grams of reactant cannot be *directly* related to the number of grams of product.

• To get grams of product from grams of reactant:

• convert grams of reactant to moles of reactant (use molar mass),

• convert moles of one reactant to moles of other reactants and products (use the stoichiometric ratio from the balanced chemical equation), and then

• convert moles back into grams for desired product (use molar mass).

Limiting Reactants

• It is not necessary to have all reactants present in stoichiometric amounts.

• Often, one or more reactants is present in excess.

• Therefore, at the end of reaction those reactants present in excess will still be in the reaction mixture.

• The one or more reactants that are completely consumed are called the **limiting reactants or limiting reagents**.

• Reactants present in excess are called *excess reactants* or *excess reagents*.

• Consider 10 H2 molecules mixed with 7 O2 molecules to form water.

• The balanced chemical equation tells us that the stoichiometric ratio of H2 to O2 is 2 to 1:

2H2(*g*) + O2(*g*) → 2H2O(*l*)

• This means that our 10 H2 molecules require 5 O2 molecules (2:1).

• Since we have 7 O2 molecules, our reaction is *limited* by the amount of H2 we have (the O2 is present in excess).

• So, all 10 H2 molecules can (and do) react with 5 of the O2 molecules producing 10 H2O molecules.

• At the end of the reaction, 2 O2 molecules remain unreacted.

Theoretical Yields

• The amount of product predicted from stoichiometry, taking into account limiting reagents, is called the **theoretical yield**.

• This is often different from the *actual yield* -- the amount of product actually obtained in the reaction.

• The **percent yield** relates the actual yield (amount of material recovered in the laboratory) to the theoretical yield:

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