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Chapter 3 Stoichiometry: Ratios of Combination

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3.1 Molecular and Formula Masses

- Molecular mass (molecular weight)
 - The mass in amu's of the individual molecule
 - Multiply the atomic mass for each element in a molecule by the number of atoms of that element and then total the masses
- Formula mass (formula weight)-

– The mass in amu's of an ionic compound

Calculating Molecular Mass

- Calculate the molecular mass (Mwt) for carbon dioxide, CO₂
- Write down each element; multiply by atomic mass

$$-C = 1 \times 12.01 = 12.01$$
 amu

- O = 2 x 16.00 = 32.00 amu
- **Total**: 12.01 + 32.00 = 44.01 amu

Your Turn!

- Calculate the molecular mass or formula mass for each of the following:
 - Sulfur trioxide
 - Barium phosphate
 - Sodium nitrite
 - Acetic acid

3.2 Percent Composition of Compounds

 Calculated by dividing the total mass of each element in a compound by the molecular mass of the compound and multiplying by 100

percent by mass of an element = $\frac{n \times \text{atomic mass of element}}{\text{molecular or formula mass of compound}} \times 100\%$

% Composition

- Calculate the percent composition of iron in a sample of iron (III) oxide
- Formula: Fe₂O₃
- Calculate formula mass
 - Fe = 2 x 55.85 = **111.70 amu**
 - $-O = 3 \times 16.00 = 48.00$ amu
 - Total mass: 111.70 + 48.00 = 159.70 amu

% Composition

% by mass =
$$\frac{111.70}{159.70} \times 100 = 69.9\%$$
 Fe

What is the % oxygen in this sample? (hint :100%)

Example

Glucose $(C_6H_{12}O_6)$ What is the mass percent of each element in glucose? - For each mole of glucose, we have 6 moles of C, 12 moles H, and 6 moles O 6 C 6 x 12.01 = 72.06 amu 12 H 12 x 1.008 = 12.096 amu + **6 O** $6 \times 16.00 = 96.00 \text{ amu} +$ 180.16 amu mass percent of C = $\frac{72.06 \text{ C}}{180.16 \text{ glucose}}$ = 0.3999 x 100 = 39.99 mass %C 12.096 H mass percent of H = $\frac{180.16 \text{ glucose}}{180.16 \text{ glucose}} = 0.06714 \text{ x } 100 = 6.714 \text{ mass %H}$ 96.00 O = 0.5329 x 100 = 53.29 mass %O mass percent of O = -9 180.16 glucose

Your Turn!

Calculate the percent oxygen in a sample of potassium chlorate

• KCIO₃

3.3 Chemical Equations

- Chemical equations represent chemical "sentences"
- Read the following equation as a sentence
 - $-NH_3 + HCI \rightarrow NH_4CI$
 - "ammonia reacts with hydrochloric acid to produce ammonium chloride"

Chemical Equations

- Reactant: any species to the left of the arrow (consumed)
- Product: any species to the right of the arrow (formed)
- State symbols:
 - -(s) solid (/) liquid (g) gas
 - -(aq) water solution

Balancing Equations

 Balanced: same number and kind of atoms on each side of the equation



 $2 H_{2(g)} + O_{2(g)} \longrightarrow 2 H_2O_{(I)}$

Balancing Equations

<u>Steps for successful balancing</u>

- Change coefficients for compounds before changing coefficients for elements.(never change subscripts!)
- 2. Treat polyatomic ions as units rather than individual elements.
- 3. Count carefully, being sure to recount after each coefficient change.

• In chemical reaction, *all atoms* present in reactants must be accounted for among the products. this is the called *balanced chemical equation*



Balancing Chemical Equations

1. Write the **correct** formula(s) for the reactants on the left side and the **correct** formula(s) for the product(s) on the right side of the equation.

Ethane reacts with oxygen to form carbon dioxide and water

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

2. Change the numbers in front of the formulas (*coefficients*) to make the number of atoms of each element the same on both sides of the equation. Do not change the subscripts.

 $2C_2H_6 \quad NOT \quad C_4H_{12}$ $2H_2O \quad NOT \quad H_4O_2$

Balancing Chemical Equations



Balancing Chemical Equations



 $2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O$

remove fraction multiply both sides by 2

Double check!

 $2C_{2}H_{6} + 7O_{2} \longrightarrow 4CO_{2} + 6H_{2}O$ $4 C (2 \times 2) \qquad 4 C$ $12 H (2 \times 6) \qquad 12 H (6 \times 2)$ $14 O (7 \times 2) \qquad 14 O (4 \times 2 + 6)$

Reactants	Products
4 C	4 C
12 H	12 H
14 O	14 O

Balancing Equations

• Balance the equation representing the combustion of hexane

$$_C_6H_{14(l)} + _O_{2(g)} \rightarrow _CO_{2(g)} + _H_2O_{(l)}$$

(Hint: Make a list of all elements and count to keep track)

Balancing Equations

• Balance the equation representing the combustion of hexane

$$C_6H_{14(l)} + 7/2O_{2(g)} \rightarrow 6CO_{2(g)} + 7H_2O_{(l)}$$

Or...multiply through the entire equation to eliminate fractions

$$2C_6H_{14(l)} + 7O_{2(g)} \rightarrow 12CO_{2(g)} + 14H_2O_{(l)}$$

Chemical Equations

 Equations can represent physical changes

 $\begin{array}{l} \mathsf{KCIO}_{3(s)} \to \mathsf{KCIO}_{3(l)} \\ \text{Or chemical changes} \end{array}$

- Note the symbol for heat above the arrow
- $\mathsf{KCIO}_{3(s)} \xrightarrow{\Delta} \mathsf{KCIO}_{3(l)}$

3.4 The Mole and Molar Masses

 Balanced equations tell us what is reacting and in what relative proportions on the molecular level.

The Mole

- The unit of measurement used by chemists in the laboratory
- **The mole** is "the number equal to number of carbon **atoms** in exactly 12 grams of pure ¹²C"
- Avogadro has determined this number to be $N_A = 6.02214 \times 10^{23}$ Particle/mole
- 1 mole ${}^{12}C$ atoms = 6.022 x 10²³ atoms = 12.00g

The Mole

$$2 \operatorname{H}_{2(g)} + \operatorname{O}_{2(g)} \rightarrow 2 \operatorname{H}_2\operatorname{O}_{(l)}$$

2 molecules $H_{2(g)} + 1$ molecule $O_{2(g)} \rightarrow 2$ molecules $H_2O_{(l)}$ 2 moles $H_{2(g)} + 1$ mole $O_{2(g)} \rightarrow 2$ moles $H_2O_{(l)}$

Molar Mass

Molar mass is the mass of 1 mole of anything in grams

- Carbon = 12.0 grams/mole
- Sodium = 22.9 grams/mole
- 1 mole lithium atoms = 6.941 g of Li

For any element

atomic mass (amu) = molar mass (grams)

Molecular mass (or molecular weight) is the sum of the atomic masses (in amu) in a molecule.



For any molecule

molecular mass (amu) = molar mass (grams)

1 molecule $SO_2 = 64.07$ amu 1 mole $SO_2 = 64.07$ g SO_2

Molar Mass for Compounds

Calculate the molar mass for each of the following:

H_2O

H 2 x 1.01 g/mol = 2.02

O 1 x 16.00 g/mol = <u>16.00</u> Molar mass = 18.02 g/mol

Example

How many atoms are in 0.551 g of potassium (K) ? 1 mol K = 39.10 g K 1 mol K = 6.022 x 10²³ atoms K 0.551 g K x $\frac{1 \text{ mol K}}{39.10 \text{ g K}}$ x $\frac{6.022 \times 10^{23} \text{ atoms K}}{1 \text{ mol K}}$ =

8.49 x 10²¹ atoms K

Example

How many H atoms are in 72.5 g of C_3H_8O ?

1 mol C₃H₈O = (3 x 12) + (8 x 1) + 16 = 60 g C₃H₈O 1 mol C₃H₈O molecules = 8 mol H atoms 1 mol H = 6.022 x 10²³ atoms H

72.5 g C₃H₈O x $\frac{1 \text{ mol } C_3H_8O}{60 \text{ g } C_3H_8O}$ x $\frac{8 \text{ mol } H \text{ atoms}}{1 \text{ mol } C_3H_8O}$ x $\frac{6.022 \text{ x } 10^{23} \text{ H atoms}}{1 \text{ mol } H \text{ atoms}} =$

5.82 x 10²⁴ atoms H

Conversions between grams, moles and atoms







Interconverting mass, moles and number of particles

Determine the number of moles in 85.00 grams of sodium chlorate, NaClO₃

$$85.00 \text{ g NaClO}_{3} \times \frac{1 \text{ mole NaClO}}{106.44 \text{ g NaClO}_{3}} = 0.7986 \text{ mol NaClO}_{3}$$

Another

Determine the number of molecules in 4.6 moles of ethanol, C_2H_5OH . (1 mole = 6.022 x 10²³)

4.6 mol C₂H₅OH ×
$$\frac{6.02 \times 10^{23} \text{ molecules C H OH}}{2 5} = 2.8 \times 10^{24} \text{ molecules}$$
$$\frac{1 \text{ mol C H OH}}{2 5}$$

Another

• Determine how many H atoms are in 4.6 moles of ethanol.

$$2.8 \times 10^{24}$$
 molecules C H OH $\times \frac{6 \text{ H atoms}}{1 \text{ molecule C H OH}} = 1.7 \times 10^{25}$ atoms H

Another

 How many grams of oxygen are present in 5.75 moles of aluminum oxide, Al₂O₃?
Strategy:

Example

Determine the number of fluorine atoms in 24.24 grams of sulfur hexafluoride.
Empirical and Molecular Formulas

- <u>Empirical</u>- simplest whole-number ratio of atoms in a formula
- Molecular the "true" ratio of atoms in a formula; often a whole-number multiple of the empirical formula
- We can determine <u>empirical formulas</u> from % composition data.

Empirical and Molecular Formulas

molecular formula = (empirical formula)_n [n = integer]

molecular formula = C_6H_6 = $(CH)_6$

empirical formula = CH

If the Molar mass for any compound is known one can get the chemical or molecular formula by the following:

- 1- calculate empirical mass = \sum atomic mass
- 1- find the multiplication factor = MM/EM
- 1- molecular formula = multiplication factor x EF

Note: if MM = EM

molecular formula = empirical formula

Example

Caffeine contain **49.48 % C, 5.159% H, 28.87 % N, and 16.49 % O** by mass has a molar mass **194.2 g/mol**. Determine the molecular formula of caffeine.

Solution

Assume you have 100g of the caffeine, Then you have 49.48 g C 5.159 g H 28.87 g N 16.49 g O

- Divide by the molar mass of each element

49.48 g C

_____ = **4.12** mol C **5.12** mol H **2.06** mol N **1.03** mol O 12.01 g/mole C

Find the ratio of the moles (divide by the smallest number)

4.12	5.12	2.06	1.03		
1.03	1.03	1.03	1.03		
4 C	5 H		2 N	10	39

Continue

4 C 5 H 2 N 1 O

-The empirical formula is $C_4H_5N_2O$

- The empirical Atomic mass = 12.01 x 4 + 1.008 x 5 + 14.01 x 2 + 16 x1 = 97.08 g/mol

- The empirical Atomic mass = 97.08 g/mol

- The multiplication factor = $\frac{194.2 \text{ g/mol}}{97.08 \text{ g/mol}} = 2$

The molecular formula = $(C_4H_5N_2O)_2 = C_8H_{10}N_4O_2$

Example

- lactic acid (*M*=90.08 g/mol) contains 40.0 mass% C, 6.71 mass% H, and 53.3 mass% O.
- Determine the molecular formula

Solution

Assuming there are 100. g of lactic acid

40 g C		6.71 g H		53.3 g C	53.3 g O 16.00 g O 3.33 mol O			
12.01g C 3.33 mol C			1.008 g	1.008 g H				
			6.66 mol H				3.33 mol	
3.33	6.66	3.33						
3.33	3.33	3.33		CH ₂ O	er	$\frac{1}{2} = \frac{1}{2} = \frac{1}$		
	90.08 g/mol		→ 3	2	C ₂ H ₂ O ₂ is the			
30.03 g/mol			· U	molecular formula	41			

Empirical Formulas

- Steps for success
 - Convert given amounts to moles
 - Mole ratio (divide all moles by the smallest number of moles)
 - The numbers represent subscripts.
 - If the numbers are not whole numbers, multiply by some factor to make them whole.

Empirical Formula

 Determine the empirical formula for a substance that is determined to be 85.63% carbon and 14.37% hydrogen by mass.

3.5 Combustion Analysis

• Analysis of organic compounds (C,H and sometimes O) are carried using an apparatus like the one below



 O_2

 CO_2, H_2O

Organic Compound

Combustion Analysis

- The data given allows an empirical formula determination with just a few more steps.
- The mass of products (carbon dioxide and water) will be known so we work our way back.

Example

• Vitamin C (M=176.12g/mol) is a compound of C,H, and O. When a 1.000-g sample of vitamin C is placed in a combustion chamber and burned, the following data are obtained:

Mass of $CO_2 = 1.50 \text{ g}$

Mass of $H_2O = 0.41$ g

What is the molecular formula of vitamin C?

Solution

There are 1 mole of C per 1 mole of CO₂

1.50 g CO₂

 $\frac{100 \text{ g} \text{ CO}_2}{44.01 \text{ g/mol CO}_2} = 0.034 \text{ mole of CO}_2 \text{ Moles of C} = \text{moles of CO}_2 = 0.034 \text{ mole}$

Mass of C = Moles of C x Molar mass of C 0.034 mole of C x 12.01 g/mol = 0.409 g C

Continue



3.6 Calculations with Balanced Chemical Equations

- <u>Balanced equations</u> allow chemists and chemistry students to calculate various amounts of reactants and products.
- The coefficients in the equation are used as <u>mole ratios</u>.

Stoichiometry

- Stoichiometry- using balanced equations to find amounts
- How do the amounts compare in the reaction below?



Mole Ratios

- Many mole ratios can be written from the equation for the synthesis of urea
- Mole ratios are used as conversion factors





- 1. Write balanced chemical equation
- 2. Convert quantities of known substances into moles
- 3. Use coefficients in balanced equation to calculate the number of moles of the required quantity
- 4. Convert moles of required quantity into desired units⁵¹

Calculations with Balanced Equations

How many moles of urea could be formed from 3.5 moles of ammonia?

$$2NH_{3(g)} + CO_{2(g)} \rightarrow (NH_2)_2 CO_{(aq)} + H_2O_{(l)}$$

3.5 mol NH₃ ×
$$\frac{1 \text{ mol } (\text{NH}_2)_2 \text{CO}}{2 \text{ mol } \text{NH}_3} = 1.8 \text{ mol } (\text{NH}_2)_2 \text{CO}$$

Mass to Mass

A chemist needs 58.75 grams of urea, how many grams of ammonia are needed to produce this amount?

Strategy:

Grams \rightarrow moles \rightarrow mole ratio \rightarrow grams

 $2\mathsf{NH}_{3(g)} + \mathsf{CO}_{2(g)} \rightarrow (\mathsf{NH}_2)_2 \mathsf{CO}_{(aq)} + H_2 O_{(l)}$

$$58.75 \text{ g} (\text{NH}_2)_2 \text{CO} \times \frac{1 \text{ mol}(\text{NH}_1) \text{ CO}}{\frac{2 2}{58.06 \text{ g}(\text{NH}_1) \text{ CO}}{2 2}} \times \frac{2 \text{ mol NH}}{1 \text{ mol}(\text{NH}_1) \text{ CO}} \times \frac{17.04 \text{ g} \text{ NH}}{1 \text{ mol NH}_3} = 34.49 \text{ g} \text{ NH}_3$$

You Try!

How many grams of carbon monoxide are needed to produce 125 grams of urea?

Example

Methanol burns in air according to the equation

 $2CH_3OH + 3O_2 \longrightarrow 2CO_2 + 4H_2O$

If 209 g of methanol are used up in the combustion, what mass of water is produced?

grams $CH_3OH \longrightarrow moles CH_3OH \longrightarrow moles H_2O \longrightarrow grams H_2O$



3.7 Limiting Reactants

- Limiting reactant the reactant that is used up first in a reaction (limits the amount of product produced)
- **Excess reactant** the one that is left over

Limiting Reagents

 $2NO + 2O_2 \longrightarrow 2NO_2$

NO is the limiting reagent

O₂ is the excess reagent





Calculation involve limiting reactant

- 1. Balance the equation.
- 2. Convert masses to moles.
- 3. Determine which reactant is limiting.
- 4. Use moles of limiting reactant and mole ratios to find moles of desired product.
- 5. Convert from moles to grams.

How to calculate Limiting Reactant In one process, **124** g of AI are reacted with **601** g of Fe_2O_3 $2AI + Fe_2O_3 \longrightarrow Al_2O_3 + 2Fe$ Calculate the mass of Al₂O₃ formed? $g AI \longrightarrow mol AI \longrightarrow mol Fe_2O_3$ needed $\longrightarrow g Fe_2O_3$ needed OR $g Fe_2O_3 \longrightarrow mol Fe_2O_3 \longrightarrow mol Al needed \longrightarrow g Al needed$ $124 \text{ gAl } x - \frac{1 \text{ mol AI}}{27.0 \text{ gAl}} x - \frac{1 \text{ mol Fe}_2 \text{O}_3}{2 \text{ mol AI}} x \frac{160. \text{ g Fe}_2 \text{O}_3}{1 \text{ mol Fe}_2 \text{O}_3} = 367 \text{ g Fe}_2 \text{O}_3$ Start with 124 g Al \longrightarrow need 367 g Fe₂O₃ Have more Fe_2O_3 (601 g) so Al is limiting reagent 59

Continue

Use limiting reagent (AI) to calculate amount of product that can be formed.

$$g \text{ AI} \longrightarrow \text{mol AI} \longrightarrow \text{mol Al}_2\text{O}_3 \longrightarrow g \text{ Al}_2\text{O}_3$$

$$2\text{AI} + \text{Fe}_2\text{O}_3 \longrightarrow \text{Al}_2\text{O}_3 + 2\text{Fe}$$

$$124 \text{ g AI} \times \frac{1 \text{ mol AI}}{27.0 \text{ g AI}} \times \frac{1 \text{ mol Al}_2\text{O}_3}{2 \text{ mol AI}} \times \frac{102. \text{ g Al}_2\text{O}_3}{1 \text{ mol Al}_2\text{O}_3} = 234 \text{ g Al}_2\text{O}_3$$

Example

- When 35.50 grams of nitrogen react with 25.75 grams of hydrogen, how many grams of ammonia are produced?
- How many grams of excess reagent remain in the reaction vessel?

$$3H_{2(g)} + N_{2(g)} \rightarrow 2NH_{3(g)}$$

Moles of N₂ = $\frac{35.5 \text{ g}}{28.01 \text{g/mol}} = 1.27 \text{ mole of } N_2$
Moles of H₂ = $\frac{25.75 \text{ g}}{2.02 \text{g/mol}} = 12.75 \text{ mole of } H_2$

$$3H_{2(g)} + N_{2(g)} \rightarrow 2NH_{3(g)}$$
 Continue

1.27 mole of N_2 12.75 mole of H_2

- 1- Assume the N_2 is the limiting reactant
- 2- Calculate how many moles of H_2 needed

Moles of H₂ needed = moles of N₂ × $\frac{3 \text{ Moles of H}_2}{1 \text{ Moles of N}_2}$ 1.27 mole N₂ × $\frac{3 \text{ Moles of H}_2}{-----}$ = **3.81 mole H**₂

1 Moles of N_2

N₂ is the limiting reactant

Continue

 $3H_{2(g)} + N_{2(g)} \rightarrow 2NH_{3(g)}$

 $g N_2 \rightarrow moles N_2 \rightarrow moles NH_3 \rightarrow g NH_3$

Moles of NH₃ = 1.27 mole N₂ × $\frac{2 \text{ Moles of NH}_3}{1 \text{ Moles of N}_2}$ = 2.54 mole NH₃

Mass of $NH_3 = 2.54$ mole × 17.03 g/mole = 43.25 g

Moles of H_2 unreacted = 12.75 - 3.81 = 8.94 moles

Mass of H_2 remains = 8.94 mole × 2.02 g/mole = 18.06 g H_2

Reaction Yield

- **Theoretical yield**: the maximum amount of product predicted by stoichiometry
- Actual yield: the amount produced in a laboratory setting
- **Percent yield**: a ratio of actual to theoretical (tells efficiency of reaction)

% Yield =
$$\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

Example

3.75 g of zinc (Zn) reacted with **excess** hydrochloric acid (HCl), **5.58** g of zinc chloride (ZnCl₂) were collected. What is the percent yield for this reaction?

$$Zn_{(s)} + 2 HCI_{(aq)} \rightarrow ZnCI_{2(aq)} + H_{2(g)}$$

g of Zn \rightarrow moles of Zn \rightarrow moles of ZnCl₂ \rightarrow g of ZnCl₂

3.75 g of Zn X
$$\underline{\text{mole}}_{65.38 \text{ g}}$$
 X $\frac{1 \text{ mole of ZnCl}_2}{1 \text{ mole of Zn}}$ X $\frac{136.3 \text{ g ZnCl}_2}{\text{mole}}$

= 7.82 g of ZnCl₂ (Theoretical Yield)

Continue

Theoretical yield = 7.82 g ZnCl₂

Actual yield = $5.58 \text{ g } \text{ZnCl}_2$



A Few Reaction Types

- **Combination**: one product is formed
- **Decomposition**: one reactant produces more than one product
- **Combustion**: a hydrocarbon reacts with oxygen to produce carbon dioxide and water

Combination Reaction

General formula: $A + B \rightarrow AB$ Sodium + chlorine \rightarrow sodium chloride $2Na + Cl_2 \rightarrow 2 NaCl$ Sulfur dioxide + water \rightarrow sulfurous acid $SO_2 + H_2O \rightarrow H_2SO_3$

Decomposition Reaction

General formula: $AB \rightarrow A + B$

Copper (II) carbonate decomposes with heat into copper (II) oxide and carbon dioxide

$$CuCO_3 \rightarrow CuO + CO_2$$

Potassium bromide decomposes into its elements

 $2\text{KBr} \rightarrow 2\text{K} + \text{Br}_2$

Combustion (hydrocarbons)

General formula: $C_xH_y + O_2 \rightarrow CO_2 + H_2O$ Methane gas burns completely $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ Butane liquid in a lighter ignites $2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$

Review

- Molecular mass
- Percent composition
- Chemical equations
 - Reactants
 - Products
 - State symbols
 - Balancing

Review continued

- Mole concept and conversions
- Empirical and molecular formulas
 - Combustion analysis
- Stoichiometry
- Limiting reactant
- % yield
- Types of reactions