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Chapter 3 Stoichiometry: Ratios of Combination

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 Molar Mass

- Calculate the molar mass 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 molar mass for each of the following:
 - Sulfur trioxide
 - Barium phosphate
 - Silver nitrate
 - Acetic acid

3.2 Percent Composition of Compounds

- Calculate by dividing the total mass of each element in a compound by the molecular mass of the compound and multiplying by 100
- % composition allows verification of purity of a sample

% Composition

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%)

Your Turn!

 Calculate the percent oxygen in a sample of potassium chlorate

3.3 Chemical Equations

- Chemical equations represent chemical "sentences"
- Read the following equation as a sentence
 - $-\operatorname{NH}_3 + \operatorname{HCI} \rightarrow \operatorname{NH}_4 \operatorname{CI}$
 - "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

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



Steps for successful balancing

- 1. 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.

 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)

 Balance the equation representing the combustion of hexane

$$C_6H_{14(l)} + 19/2O_{2(g)} \rightarrow 6CO_{2(g)} + 7H_2O_{(l)}$$

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

$$2C_6H_{14(l)} + 19O_{2(g)} \rightarrow 12CO_{2(g)} + 14H_2O_{(l)}$$

Chemical Equations

Equations can represent physical changes: $KCIO_{3(s)} \rightarrow KCIO_{3(l)}$

Or chemical changes:

2 KCIO_{3(s)}

• Note the symbol for heat above the arrow $\xrightarrow{\Delta}$

$$2 \text{ KCI}_{(s)} + 3 \text{ O}_{2(g)}$$

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3.4 The Mole and Molar Masses

- Balanced equations tell us what is reacting and in what relative proportions on the molecular level.
- However, chemists must work with the chemical reactions on a macroscopic level.

The Mole

- The unit of measurement used by chemists in the laboratory
- 1 mole = 6.022×10^{23}
 - (Avogadro's number represents the number of atoms that exist in exactly 12 grams of carbon-12)
 - This is our "counting number" for atoms, molecules and ions much like a dozen is our counting number for cookies or doughnuts)

The Mole

$$2 H_{2(g)} + O_{2(g)} \rightarrow 2 H_2 O_{(l)}$$

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 $H_2O_{(l)}$

This relationship can be made because of Avogadro's number (N_A)

Moles and Atoms



- Calculate the number of atoms found in 4.50 moles of silicon.
- How many moles of silicon are in 2.45 x 10⁴⁵ atoms?

 $N_{\rm A}$ = Avogadro's number

Molar Mass

- Molar mass the mass of one mole of a substance in grams
- Carbon = 12.0 grams/mole
- Sodium = 22.9 grams/mole

 What is the relationship between molar mass and atomic mass?

Molar Mass

- What is molar mass for each of the following?
- Copper metal =
- Helium gas =
- Calcium metal =

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

Your Turn!

Calculate the molar mass for each of the following: Carbon dioxide Ammonia Oxygen gas

(Don't forget the diatomics!)

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

Another

- Determine how many H atoms are in 4.6 moles of ethanol.
 - Begin with the answer to the last problem

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

Your Turn

Solve the following conversions

How many atoms of silver are in 3.50 moles of silver?

- Determine the number of moles of carbon disulfide in 34.75 grams of CS₂.
- Determine the number of sulfur atoms in 34.75 grams of CS₂.

Another

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

Challenge

Determine the number of fluorine atoms in 24.24 grams of sulfur hexafluoride. (hint: make a plan first!)

Empirical and Molecular Formulas

- Empirical- 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 empirical formulas from % composition data; a good analysis tool.

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.

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



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- 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.

Suppose that 18.8 grams of glucose was burned in a combustion train resulting in 27.6 grams of carbon dioxide and 11.3 grams of water. Calculate the empirical and molecular formula of glucose. Molar mass = 180 g/mol (Assumptions: all C in CO₂ originates from glucose; all H in H₂O originates from glucose; O is found by difference)

Steps:

Convert 27.6 g CO_2 into g of C Convert 11.3 g H_2O into g H Calculate g O = g sample - (g C + g H) Find empirical formula as before (g to moles, mole ratio)

Molecular formula

- = molecular mass/empirical mass
- = 180/30 = 6

Multiply through empirical formula to obtain new subscripts

Molecular formula = $C_6H_{12}O_6$

3.6 Calculations with Balanced Chemical Equations

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

Stoichiometry

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



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Mole Ratios

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



Calculations with Balanced Equations

 How many moles of urea could be formed from 3.5 moles of ammonia?
 2NH_{3(g)}+ CO_{2(g)} → (NH₂)₂CO_(aq)+ H₂O_(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

$$58.75 \text{ g (NH}_{2})_{2} \text{CO} \times \frac{1 \text{ mol(NH}) \text{ CO}}{\frac{2 2}{58.06 \text{ g (NH}) 2 2}} \times \frac{2 \text{ mol NH}}{1 \text{ mol (NH}) 2 2} \times \frac{17.04 \text{ g NH}}{1 \text{ mol NH} 3} = 34.49 \text{ g NH}_{3}$$

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Correction to the publisher's prevous slide:

MW urea 60.06 g/mol

So mass is 33.34g.

You Try!

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

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
 - Industry often makes the more expensive reactant the limiting one to ensure its complete conversion into products

- If one loaf of bread contains 16 slices of bread and a package of lunchmeat contains 10 slices of turkey, how many sandwiches can be made with 2 pieces of bread and one slice of meat?
- Which is the limiting reactant? How much excess reactant is left?

How do you identify a limiting reactant problem?

Example:

If 5.0 moles of hydrogen react with 5.0 moles of oxygen, how many moles of water can be produced?

Notice: both reactant amounts are given and a product amount is requested

Steps for Success

- Step 1: write a balanced equation
- Step 2: identify the limiting reactant
 Must compare in terms of moles
- Step 3: use a mole ratio to desired substance
- Step 4: convert to desired units

How many molecules of water are formed when 7.50 grams of hydrogen gas react with 5.00 grams of oxygen gas?

Step 1: $2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(/)}$ Step 2: 7.50 g H₂/2.02 g/mol = 3.712 mol 5.00 g O₂ / 32.00 g/mol = 0.1562 mol

Step 2 continued:

Decide which is limiting - look at the mole ratio of reactants--it takes twice as much $H_2 as O_2$ so O_2 limits in this case.

Step 3 and step 4:



 In the previous example, how many grams of hydrogen were left in excess?
 Step 1: how much H₂ is used

$$0.1562 \text{ molO}_2 \times \frac{2 \text{ molH}}{1 \text{ molO}_2} \times \frac{2.02 \text{ g H}}{2} = 0.63104 \text{ g H}_2 \text{ used}$$

In the previous example, how many grams of hydrogen were left in excess?
 Step 2: initial H₂ - used H₂
 7.50 g - 0.63 g = 6.87 g excess

Your Turn!

- 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?

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)

Percent Yield

When a student reacted 3.75 grams of zinc with excess hydrochloric acid, 1.58 grams of zinc chloride were collected. What is the percent yield for this reaction?

% yield =
$$\frac{\text{actual}}{\text{theoretical}} \times 100$$

Percent Yield

- Step 1: Balanced equation
- Step 2: Calculate theoretical yield
- Step 3: Substitute into formula and solve

Percent Yield

 $Zn_{(s)} + 2 HCI_{(aq)} \rightarrow ZnCI_{2(aq)} + H_{2(g)}$ Theoretical yield = 7.82 g $ZnCI_2$ Actual yield = 1.58 g $ZnCI_2$

Calculate % yield:

(1.58g/7.82g)x100% = 20.2%

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