

Chapter 3

Stoichiometry

Ratios of combination

Topics

- **Molecular and formula masses**
- **Percent composition of compounds**
- **Chemical equations**
- **Mole and molar mass**
- **Combustion analysis (Determining the formula of a compound)**
- **Calculations with balanced chemical equations**
- **Calculations involving limiting reactant**

Chemical Stoichiometry

- **Stoichimetry** from Greek “measuring elements”.

That is “Calculation of quantities in chemical reactions”

- **Stoichiometry** - The study of quantities of materials **consumed** and **produced** in chemical reactions.

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 one formula unit of an **ionic compound**

Calculating the molecular mass

- Calculate the molecular mass for carbon dioxide, CO_2
- Write down each element; multiply by atomic mass
 - C = 1 x 12.01 = 12.01 amu
 - O = 2 x 16.00 = 32.00 amu

 - Total: 12.01 + 32.00 = 44.01 amu

Calculating the formula mass

- Calculate the formula mass for sodium nitrate, NaNO_3
- Write down each element; multiply by atomic mass
 - Na = 1 x 23.0 = 23.0 amu
 - N = 1 x 14.01 = 14.01 amu
 - O = 3 x 16.0 = 48.0 amu

 - Total: 23.0 + 14.01 + 48.0 = 85.01 amu

3.2 Percent Composition of Compounds

- % composition is calculated 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**

Percent Composition of Compounds

$$\frac{n \times \text{atomic mass of element}}{\text{Molecular or formula mass of compound}} \times 100\%$$

% Composition

- Calculate the percent composition of iron in a sample of iron (III) oxide
- Formula: Fe_2O_3
- Calculate formula mass
 - Fe = $2 \times 55.85 = 111.70$ amu
 - O = $3 \times 16.00 = 48.00$ amu
 - Total mass: $111.70 + 48.00 = 159.70$ amu

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

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

% Composition

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

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

Practice

Find the percent composition of each element in $\text{C}_2\text{H}_6\text{O}$

$$\%C = \frac{2 \times (12.01 \text{ g})}{46.07 \text{ g}} \times 100\% = 52.14\%$$

$$\%H = \frac{6 \times (1.008 \text{ g})}{46.07 \text{ g}} \times 100\% = 13.13\%$$

$$\%O = \frac{1 \times (16.00 \text{ g})}{46.07 \text{ g}} \times 100\% = 34.73\%$$

$$52.14\% + 13.13\% + 34.73\% = 100.0\%$$

3.3 Chemical Equations

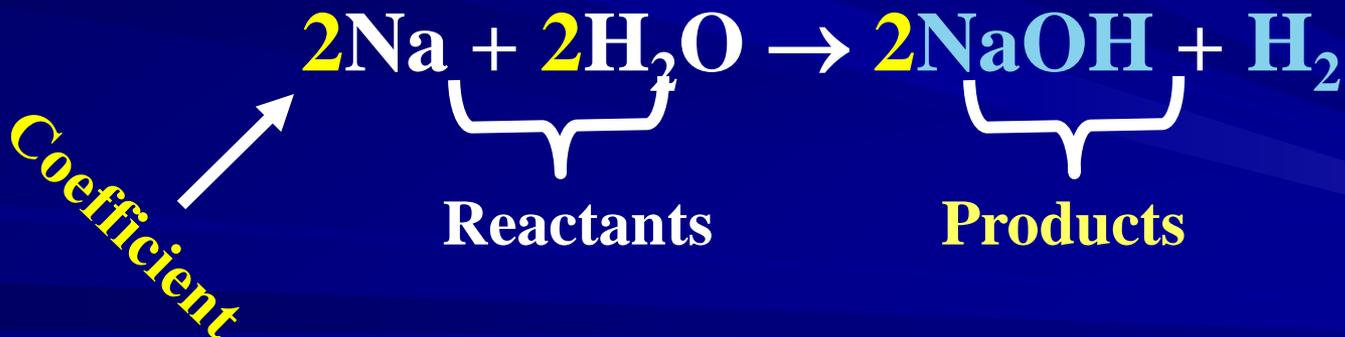
- Chemical equations represent chemical “**sentences**”
- Read the following equation as a sentence
 - $\text{NH}_3 + \text{HCl} \rightarrow \text{NH}_4\text{Cl}$
 - “ammonia reacts with hydrochloric acid to produce ammonium chloride”

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 (l) liquid (g) gas
 - (aq) water solution

Reading Chemical Equations

- The plus sign (+) means “react” and the arrow points towards the substance produced in the reaction.
- The chemical formulas on the left side of the equation are called **reactants (consumed)** and after the arrow (right side) are called **products (formed)**.
- The numbers in front of the formulas are called **stoichiometric coefficients**.



- **Stoichiometric coefficients:** numbers in front of the chemical formulas; give ratio of reactants and products.

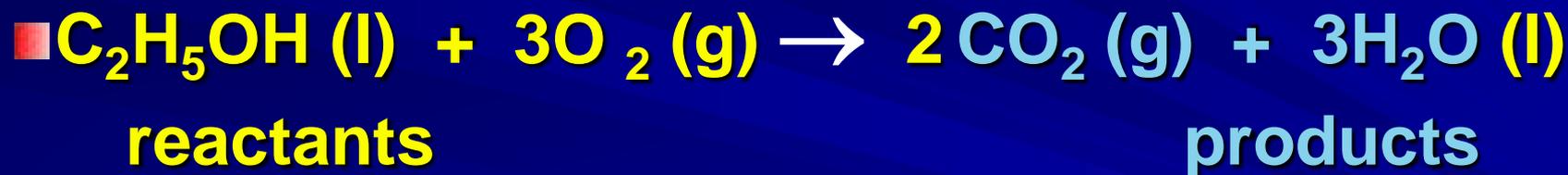
Chemical Equations

■ A representation of a chemical reaction:

■ **State symbols:**

– (s) solid (l) liquid (g) gas

– (aq) water solution



Catalysts, photons ($h\nu$), or heat (Δ) may stand above the reaction arrow (\rightarrow).

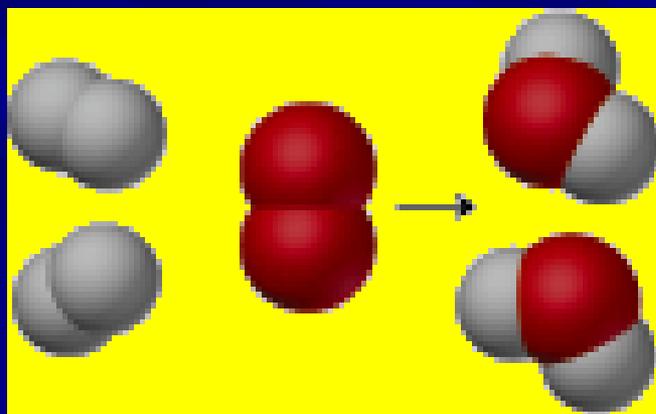
Balanced chemical equation



■ The equation is balanced.

■ 1 molecule of ethanol reacts with 3 molecules of oxygen to produce 2 molecules of carbon dioxide and 3 molecules of water

- The chemical equation for the formation of water can be visualized as two hydrogen molecules reacting with one oxygen molecule to form two water molecules:



Products

Reactants

Chemical Equations

- Equations can represent **physical changes**



Or **chemical changes**

- Note the symbol for heat above the arrow



Balancing chemical equations

- When balancing a chemical reaction coefficients are added in front of the compounds to balance the reaction, **but subscripts should not be changed**
- **Changing the subscripts changes the compound**

Balancing Equations

■ Steps for successful balancing

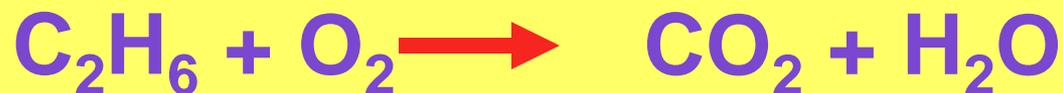
1. Change coefficients for **compounds** before changing coefficients for **elements**. (never change subscripts!)
2. Treat **polyatomic ions as units** rather than individual elements.
3. **Count carefully**, being sure to recount after each coefficient change.

Balancing Chemical Equations

By inspection (Trial and error)

- ❖ 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



- ❖ 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.



Balancing Chemical Equations

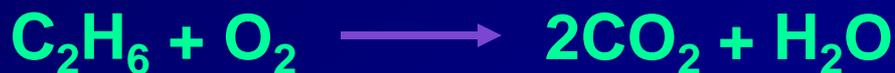
- ❖ Start by balancing those elements that appear in only one reactant and one product.



2 carbon
on left

1 carbon
on right

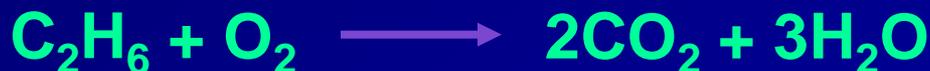
multiply CO_2 by 2



6 hydrogen
on left

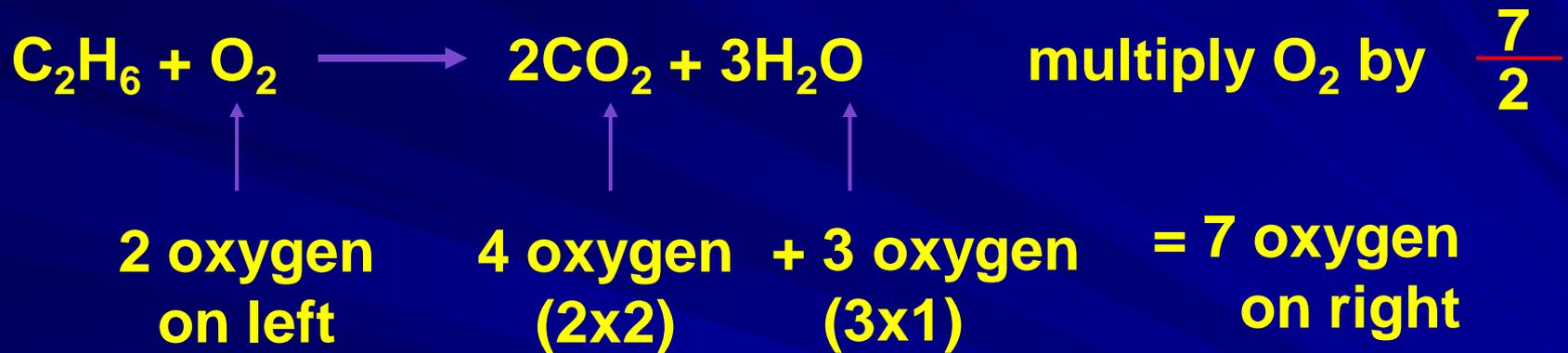
2 hydrogen
on right

multiply H_2O by 3



Balancing Chemical Equations

- ❖ Balance those elements that appear in two or more reactants or products.



Balancing Chemical Equations

- ❖ Check to make sure that you have the same number of each type of atom on both sides of the equation.



4 C (2 x 2)

4 C

12 H (2 x 6)

12 H (6 x 2)

14 O (7 x 2)

14 O (4 x 2 + 6)

Balancing Chemical Equations

- ❖ Check to make sure that you have the same number of each type of atom on both sides of the equation.



<u>Reactants</u>	<u>Products</u>
4 C	4 C
12 H	12 H
14 O	14 O

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 *mole (mol)* is a number equal to the number of carbon atoms in exactly 12.00 grams of ^{12}C (Counting by weight??)
- Techniques such as mass spectrometry were used to count this number
- The number was found as 6.02214×10^{23}
- This number was known as “Avogadro’s number”
- Thus, one mole of a substance contains of 6.022×10^{23} units of that substance
- So, as a dozen of eggs is 12; a mole of eggs is Avogadro’s number of eggs.

The Mole



2 molecules $\text{H}_{2(g)}$ + 1 molecule $\text{O}_{2(g)}$ \rightarrow 2 molecules $\text{H}_2\text{O}_{(l)}$

2 moles $\text{H}_{2(g)}$ + 1 mole $\text{O}_{2(g)}$ \rightarrow 2 moles $\text{H}_2\text{O}_{(l)}$

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

How the mole is used in chemical calculations?

- 12 grams of ^{12}C contain Avogadro's number of atoms
= 6.022×10^{23} C atoms
- 12.01 g of natural C (^{12}C , ^{13}C , ^{14}C) contains 6.022×10^{23} C atoms
- Atomic mass of C atom = 12.01 amu

Express amu in grams

6.022×10^{23} atoms of C (each has a mass of 12 amu) have a mass of 12 g

$$? \text{ g in} = 6.022 \times 10^{23} \text{ amu} \times \frac{1 \text{ C atom}}{12 \text{ amu}} \times \frac{12 \text{ g}}{6.022 \times 10^{23} \text{ C atoms}} = 1 \text{ g}$$

Avogadro's number of amu = 1 g C

Moles and Atoms

Number of moles

Multiply by N_A

Divide by N_A

**Number of atoms, molecules,
or formula units**

$N_A = \text{Avogadro's number}$

Molar mass

- Molar mass is the mass of 1 mole of a substance expressed in grams.
- Often called **molecular weight**.
- To determine the molar mass of a compound: **add up the molar masses of the elements (taking # moles of each element into consideration) that makes it up.**

Molar Mass

- Molar masses of elements:

Carbon = 12.0 grams/mole

Sodium = 22.9 grams/mole

- What is the relationship between molar mass and atomic mass?

Molar Mass for Compounds

Calculate the molar mass for each of

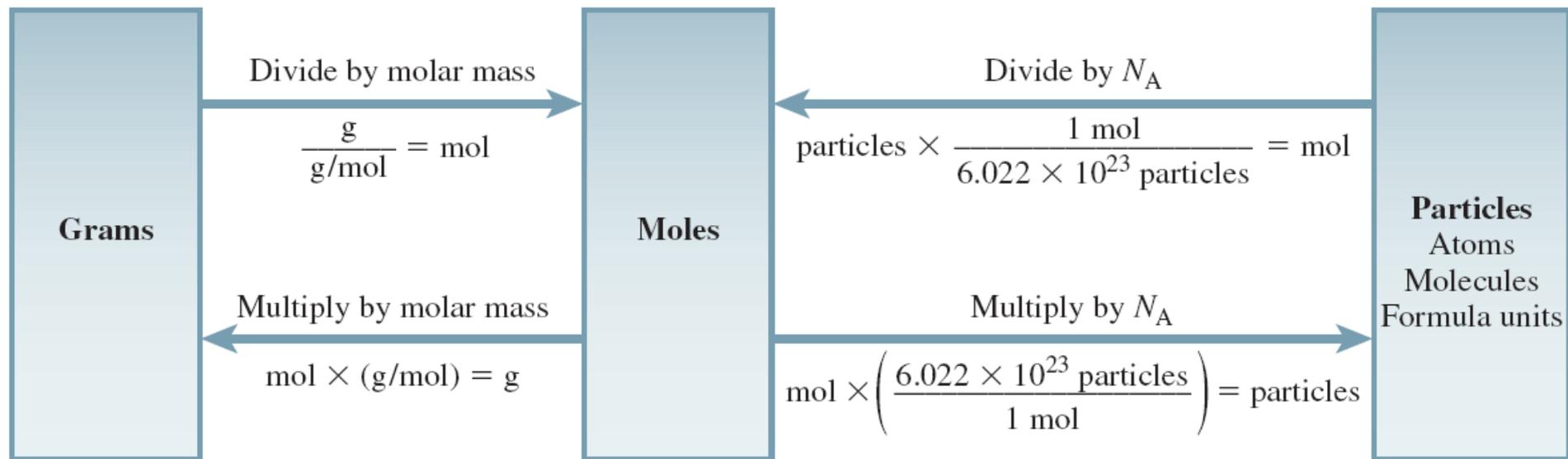


$$\text{H } 2 \times 1.01 \text{ g/mol} = 2.02$$

$$\text{O } 1 \times 16.00 \text{ g/mol} = \underline{16.00}$$

$$\text{Molar mass} = 18.02 \text{ g/mol}$$

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, NaClO_3

$$85.00 \text{ g NaClO}_3 \times \frac{1 \text{ mole NaClO}_3}{106.44 \text{ g NaClO}_3} = 0.7986 \text{ mol NaClO}_3$$

Example

Determine the number of molecules in 4.6 moles of ethanol, C₂H₅OH.

(1 mole = 6.022 × 10²³)

$$4.6 \text{ mol C}_2\text{H}_5\text{OH} \times \frac{6.02 \times 10^{23} \text{ molecules C}_2\text{H}_5\text{OH}}{1 \text{ mol C}_2\text{H}_5\text{OH}} = 2.8 \times 10^{24} \text{ molecules}$$

Empirical and Molecular Formulas

Empirical formula: the lowest whole number ratio of atoms in a compound.

Molecular formula: the true number of atoms of each element in the formula of a compound.

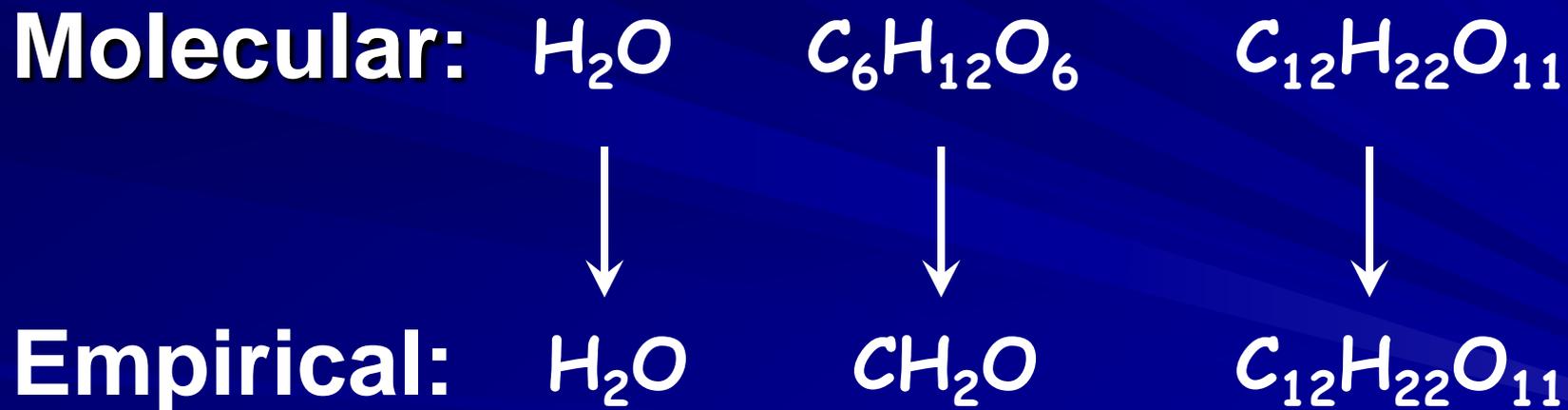
- molecular formula = (empirical formula)_n
- [n = integer]
- molecular formula = C₆H₆ = (CH)₆
- empirical formula = CH

Formulas for **ionic compounds** are **ALWAYS** empirical (lowest whole number ratio).

Examples:



Formulas for **molecular compounds** **MIGHT** be empirical (lowest whole number ratio).



Calculating Empirical Formula from percent composition

- Empirical formulas can be determined from % composition data; a good analysis tool.
- Assume you have a 100 g. Then the percentages become grams.
- Convert grams to moles
- Find the 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.*

Example

■ Calculate the empirical formula of a compound composed of 38.67 % C, 16.22 % H, and 45.11 %N.

■ Assume 100 g so

$$\text{■ } 38.67 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ gC}} = 3.220 \text{ mole C}$$

$$\text{■ } 16.22 \text{ g H} \times \frac{1 \text{ mol H}}{1.01 \text{ gH}} = 16.09 \text{ mole H}$$

$$\text{■ } 45.11 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ gN}} = 3.219 \text{ mole N}$$

Now divide each value by the smallest value

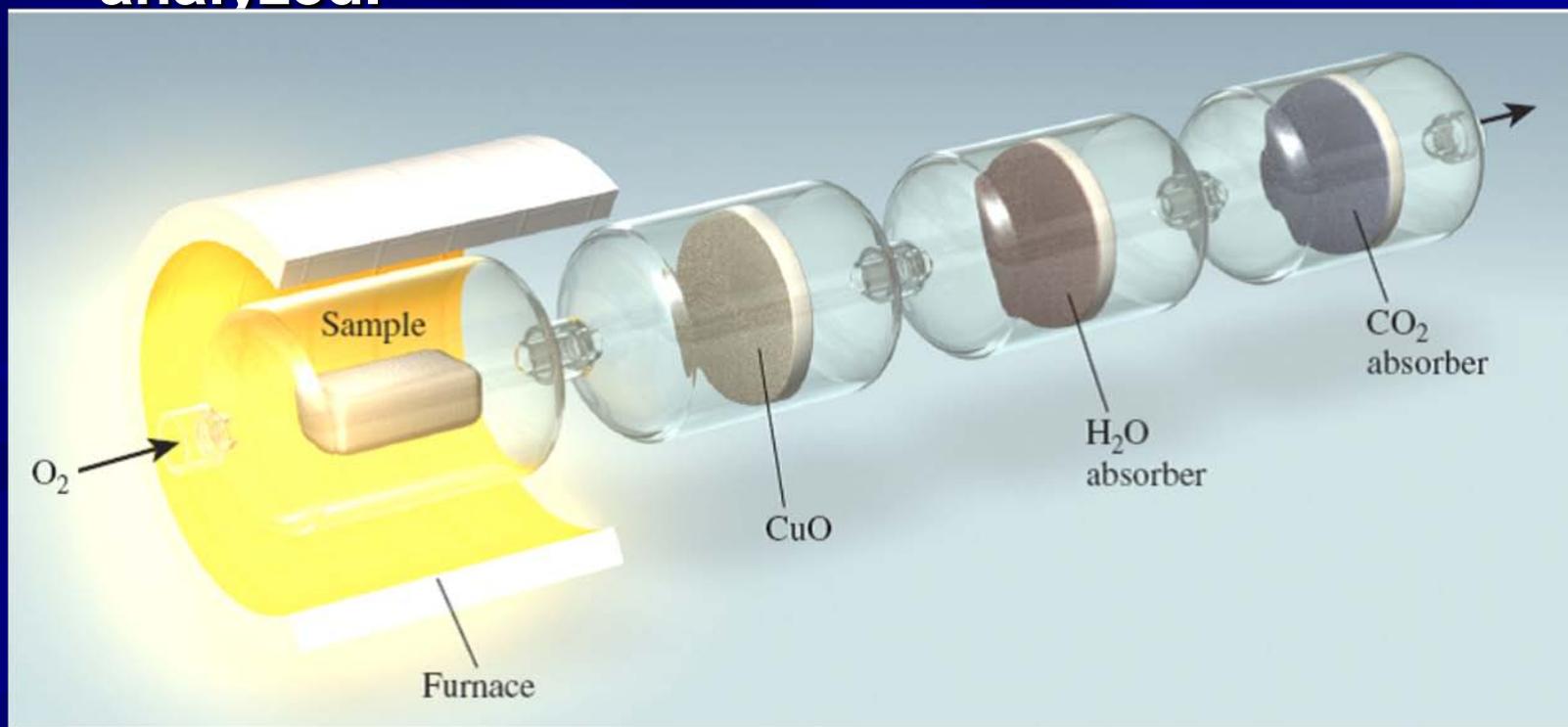
■ The ratio is $\frac{3.220 \text{ mol C}}{3.219 \text{ mol N}} = \frac{1 \text{ mol C}}{1 \text{ mol N}}$

■ The ratio is $\frac{16.09 \text{ mol H}}{3.219 \text{ mol N}} = \frac{5 \text{ mol H}}{1 \text{ mol}}$



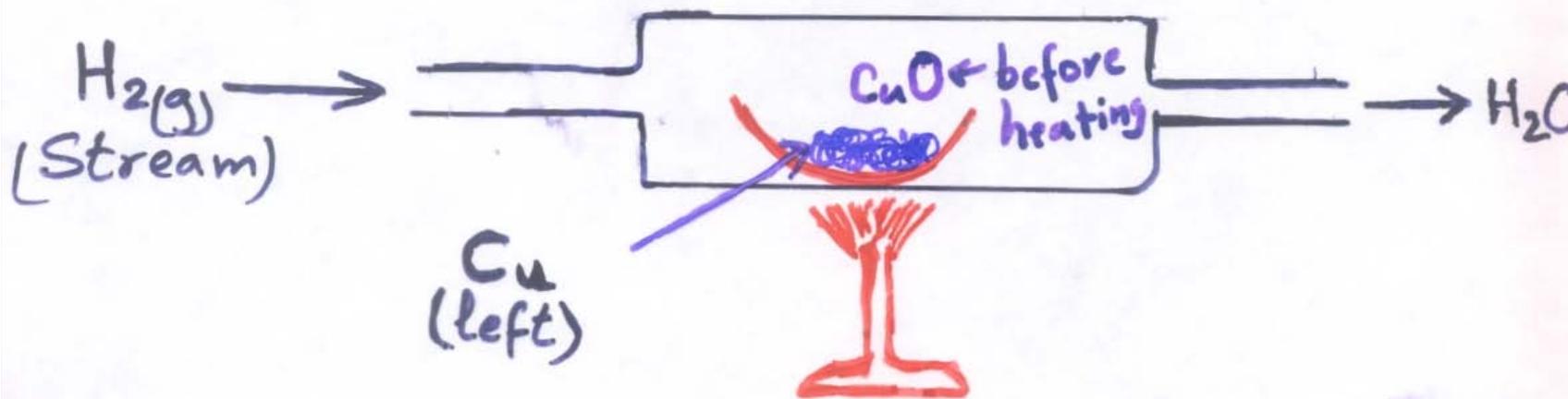
3.5 Combustion Analysis

- Analysis of organic compounds (C,H and sometimes O) are carried using an apparatus like the one below
- A compound of unknown composition is decomposed by heat. The elements are carefully trapped and the number of moles of each are analyzed.

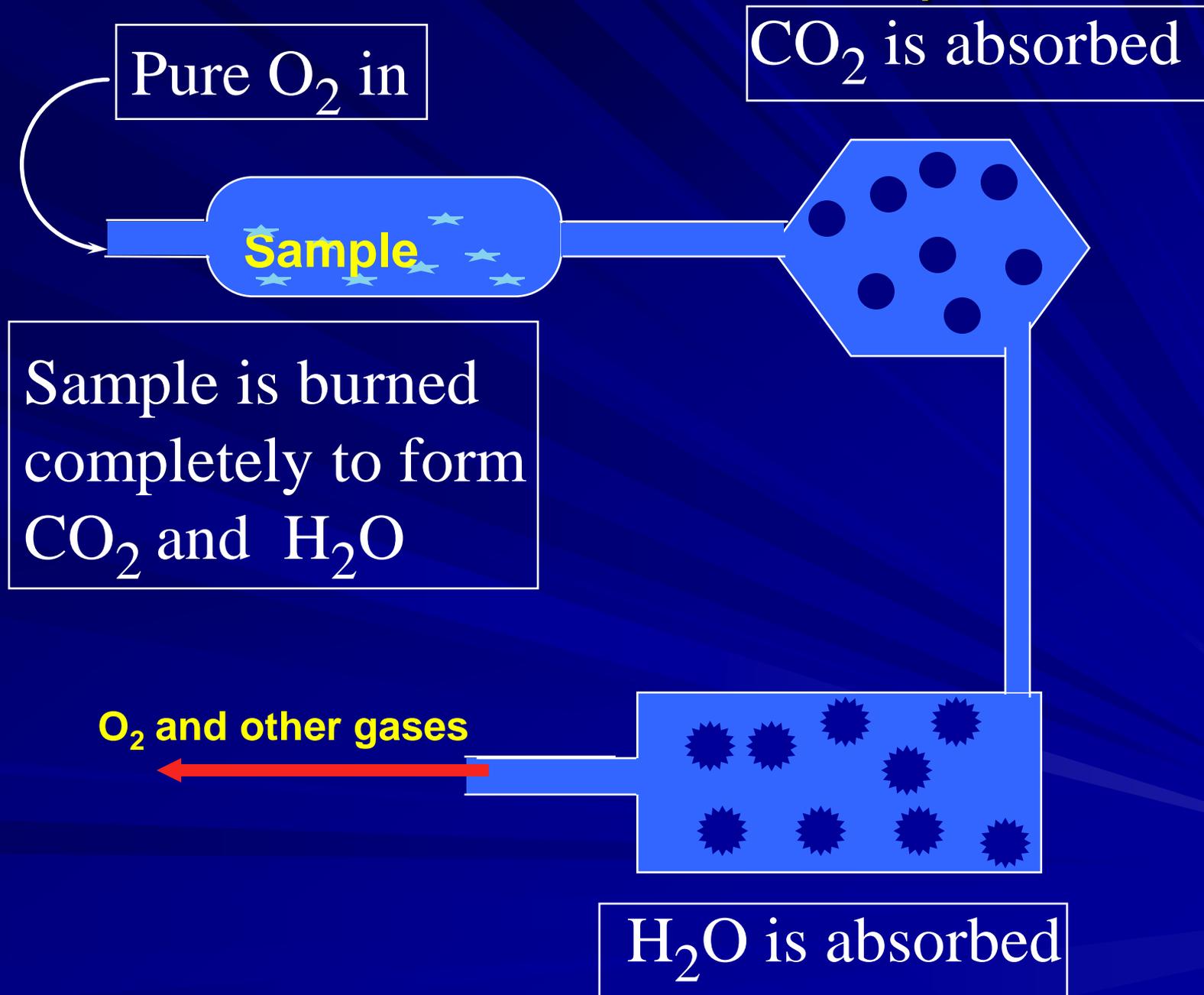


Determination of percent composition and simplest formula from experiment

e.g Oxides of some metal ions



Experimental Determination of the formula of a compound



Experimental Determination of the formula of a compound by elemental analysis

- A sample of a compound composed of carbon oxygen and hydrogen are combusted in a stream of O_2 to produce CO_2 and H_2O . The H_2O and CO_2 are trapped and the masses of each are measured.

Calculating empirical formula

A sample of certain material contains only C, H and O has a mass of 0.255g. When the reaction is complete, 0.561 g of CO₂ and 0.306g of H₂O are produced. **What is the empirical formula of the compound?**

1. Determine the mass of C in the sample.

- For each mole of CO₂, there is one mole of C. **Convert moles of C to grams of C.**
- $0.561 \text{ g CO}_2 \times (1 \text{ mol CO}_2 / 44.01 \text{ g CO}_2) \times (1 \text{ mol C} / 1 \text{ mol CO}_2) (12.01 \text{ g C} / \text{mol C})$
 $= 0.153 \text{ g C}$

2. Determine the mass of H in the sample.

- There are 2 moles of hydrogen per mole of H_2O .
- $0.306 \text{ g H}_2\text{O} \times (1 \text{ mol H}_2\text{O} / 18.0 \text{ g H}_2\text{O}) \times (2 \text{ mole H} / \text{mole H}_2\text{O}) \times (1.01 \text{ g H} / \text{mol H}) = 0.0343 \text{ g H}$

3. *Mass O = mass sample - mass H - mass C*

- Mass sample = 0.255 g
- Mass O = $0.255 - 0.153 - 0.0343 = 0.068 \text{ g O}$

- To get empirical formula, convert g back to moles
- $0.153 \text{ g C} \times (1 \text{ mol C} / 12.01 \text{ g C}) = 0.0128 \text{ mol C}$
- $0.0343 \text{ g H} \times (1 \text{ mol H} / 1.01 \text{ g H}) = 0.0340 \text{ mol H}$
- $0.068 \text{ g O} \times (1 \text{ mol O} / 16.0 \text{ g O}) = 0.0043 \text{ mol O}$
- Divide each by **0.0043** to get ratio of each element to O
- **C:** $0.0128 \text{ mol C} / 0.0043 \text{ mol O} = 2.98 \sim 3$
- There are 3 moles of carbon for each mole of oxygen
- **H:** $0.0340 \text{ mol H} / 0.0043 \text{ mol O} = 7.91 \sim 8$
- There are 8 moles of hydrogen per mole of oxygen
- Empirical Formula **$\text{C}_3\text{H}_8\text{O}$**

Determining **molecular** formula from empirical formula

- Since the empirical formula is the lowest ratio, the actual molecule would weigh more.
 - **By a whole number multiple.**
- Divide the **actual molar mass** by the **empirical formula mass**

■ Benzene has the empirical formula CH and a molar mass of 78.0 g. what is its molecular formula?

Empirical formula mass = $12.0 + 1.00 = 13.00$ g/mol

■ $n = \text{actual molar mass} / \text{empirical formula mass}$

■ $n = 78.0 / 13.0 = 6$

■ molecular formula = (empirical formula)_{*n*}
n = integer]

■ molecular formula = C₆H₆

Example

A 2.103 g Copper oxide when heated in a stream of $H_2(g)$ yields 0.476 g H_2O .

What is the formula of copper oxide

Mass of O in H_2O formed = mass of O in the oxide

$$\#g O = 0.476 g H_2O \times \frac{16g O}{18.0g H_2O} = 0.423g O$$

$$\text{Mass of Cu} = 2.103g - 0.423g = 1.680g$$

$$\# \text{ mol O} = 0.423 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.0264 \text{ mol}$$

$$\begin{aligned} \# \text{ mol Cu} &= 1.680 \text{ g Cu} \times \frac{1 \text{ mol Cu}}{63.55 \text{ g Cu}} \\ &= 0.0264 \text{ mol} \end{aligned}$$

The Simplest ratio of O : Cu is

$$0.0264 \text{ mol O} : 0.0264 \text{ mol Cu}$$

$$\frac{0.0264 \text{ mol O}}{0.0264} : \frac{0.0264 \text{ mol Cu}}{0.0264}$$



\therefore The Simplest formula of
Copper oxide is CuO

If the Simplest mole ratio involves
one or more fractional numbers

e.g : $3.50 : 2.33$

Multiply through by the Smallest
integer that will give Whole number
ratio

$$\frac{3.50 \times \frac{2}{2}}{2.33 \times \frac{3}{3}} = \frac{7/2}{6.99/3} \approx \boxed{\frac{3}{2}}$$

3.6 Calculations with balanced chemical equations

- Chemical reactions involve changes in matter, making of new materials with new properties, or energy changes.
- Atoms cannot be created or destroyed
- Chemical reactions are described using the chemical equations
- Given an amount of either starting material or product, other quantities can be determined.
- use conversion factors from
 - molar mass (g - mole)
 - balanced equation (mole - mole)

Calculations of moles of reactants or products from Balanced Equations

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



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

Calculations of mass of reactants or products from Balanced Equations

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



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

Example



If we have 15.0 g of C_2H_4 **how many moles of HCl** are needed to carry out the reaction to completion?

The balanced equation tells us it takes 1 mole of HCl for each mole of C_2H_4 reacted.

We must begin by converting the number of grams of C_2H_4 which has a molar mass of 28.08 g/mol, to moles

$$15.0 \text{ g } \cancel{\text{C}_2\text{H}_4} \times \frac{1 \text{ mol } \cancel{\text{C}_2\text{H}_4}}{28.08 \text{ g } \cancel{\text{C}_2\text{H}_4}} = 0.534 \text{ mol } \text{C}_2\text{H}_4$$

What moles of HCl is needed to carry the reaction through to completion?

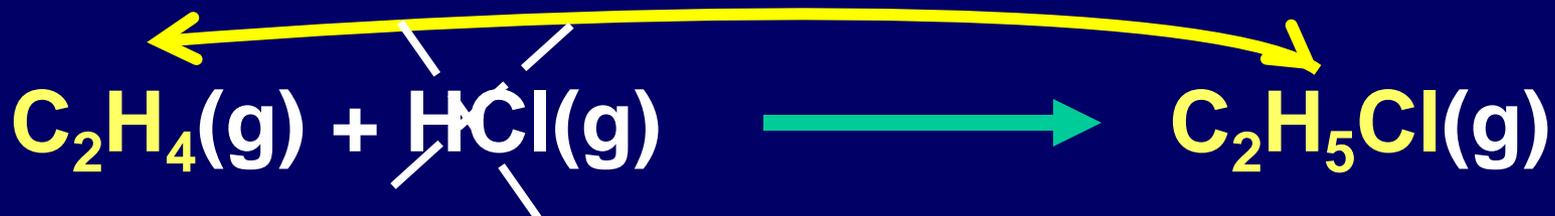


$$0.534 \text{ mol } \cancel{\text{C}_2\text{H}_4} \times \frac{1 \text{ mol HCl}}{1 \cancel{\text{mol C}_2\text{H}_4}} = 0.534 \text{ mol HCl}$$

What mass of HCl is needed to carry the reaction through to completion?

$$0.534 \text{ mol HCl} \times \frac{36.5 \text{ g HCl}}{1 \text{ mol HCl}} = 19.6 \text{ g HCl}$$

Example



How many moles of product are made when 15.0 g of C_2H_4 is reacted with an excess of HCl?



15.0 g

?

Molar mass of C_2H_4 (ethylene) = 28.08 g/mol

$$15.0 \text{ g C}_2\text{H}_4 \times \frac{1 \text{ mole C}_2\text{H}_4}{28.06 \text{ g C}_2\text{H}_4} = 0.534 \text{ mol C}_2\text{H}_4$$

Stoichiometry of the balanced equation indicates a mole ratio of 1:1 reactants



0.534 mol

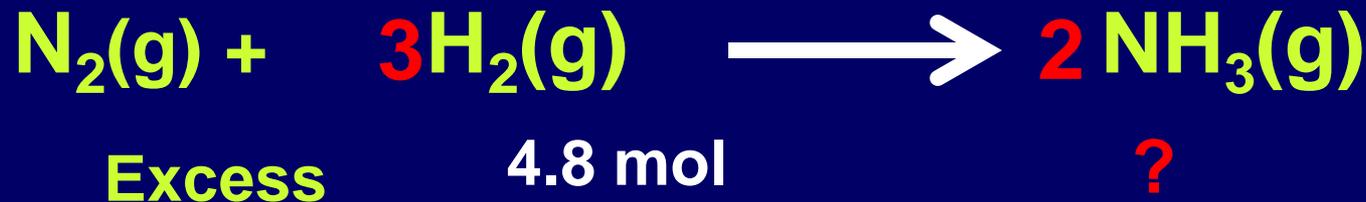
0.534 mol

(molar mass $\text{C}_2\text{H}_5\text{Cl} = 64.51 \text{ g/mol}$)

$$0.543 \text{ mol } \text{C}_2\text{H}_5\text{Cl} \times \frac{64.51 \text{ g } \text{C}_2\text{H}_5\text{Cl}}{1 \text{ mol } \text{C}_2\text{H}_5\text{Cl}} = 35.0 \text{ g } \text{C}_2\text{H}_5\text{Cl}$$

Example

How many grams of NH₃ will be produced from 4.8 mol H₂?



Begin with what you are given. You have 4.8 mol H₂

$$4.8 \text{ mol } \cancel{\text{H}_2} \times \frac{2 \text{ mol } \text{NH}_3}{3 \cancel{\text{ mol } \text{H}_2}} = 3.2 \text{ mol } \text{NH}_3$$

$$3.2 \text{ mol } \text{NH}_3 \times \frac{17.0 \text{ g } \text{NH}_3}{1 \text{ mol } \text{NH}_3} = 54.4 \text{ g } \text{NH}_3$$

3.7 Limiting reactants

- If the reactants are not present in stoichiometric amounts, at end of reaction some reactants are still present (in excess).
- **Limiting Reactant:** one reactant that is consumed

Limiting Reactant: Reactant that limits the amount of product formed in a chemical reaction

Excess reactant - the one that is left over

Limiting Reactants/ Example



when 3.5g of Cu is added to a solution containing 6.0g of AgNO₃ what is the limiting reactant?

What is the mass Ag produced and what is the mass of the excess reagent?

Calculations involving a limiting reactant



$$1. \quad 3.5\text{g Cu} \times \frac{1 \text{ mol Cu}}{63.5\text{g Cu}} \times \frac{2 \text{ mol Ag}}{1 \text{ mol Cu}} = 0.11 \text{ mol of Ag}$$

$$2. \quad 6.0\text{g AgNO}_3 \times \frac{1 \text{ mol AgNO}_3}{170\text{g AgNO}_3} \times \frac{2 \text{ mol Ag}}{2 \text{ mol AgNO}_3} = 0.035 \text{ mol Ag}$$

The Limiting Reactant is AgNO_3 .

Limiting reactant is:

The reactant that produces the least amount of product

Determining the limiting reactant by comparing the mole ratio of Cu and AgNO₃ required by the balanced equation with the mole ratio actually present



$$3.5\text{g Cu} \times \frac{1 \text{ mol Cu}}{63.5\text{g Cu}} = 0.055 \text{ mol Cu}$$

$$6.0\text{g AgNO}_3 \times \frac{1 \text{ mol AgNO}_3}{170\text{g AgNO}_3} = 0.0353 \text{ mol AgNO}_3$$

$$\text{Mole ratio required by the balanced equation} = \frac{\text{mol AgNO}_3}{\text{mol Cu}} = \frac{2}{1} = 2.0$$

$$\text{Actual mole ratio} = \frac{\text{mol AgNO}_3}{\text{mol Cu}} = 0.64$$

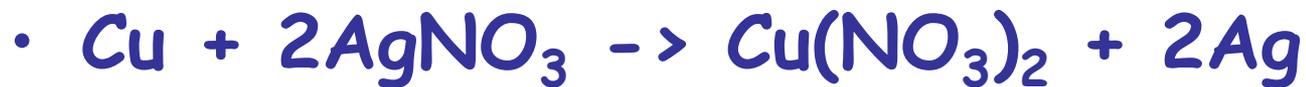
Thus AgNO₃ is the limiting reactant

What is the mass of Ag produced?

Take the limiting reactant:

$$6.0\text{g AgNO}_3 \times \frac{1\text{mol AgNO}_3}{170\text{g AgNO}_3} \times \frac{2\text{mol Ag}}{2\text{mol AgNO}_3} \times \frac{108\text{g Ag}}{1\text{mol Ag}} \\ = 3.8\text{g Ag}$$

Excess reagent



Excess reagent is ?????

Calculate amount of Cu needed to react with the limiting reactant

$$6.0\text{g AgNO}_3 \times \frac{1\text{mol AgNO}_3}{170\text{g AgNO}_3} \times \frac{1\text{mol Cu}}{2\text{mol AgNO}_3} \times \frac{63.5\text{ Cu}}{1\text{molCu}} \\ = 1.12 \text{ g Cu}$$

Amount of Cu left (Excess reagent) = 3.5 – 1.12 = 2.38 g Cu

The Reaction Yield

- The amount of stuff you make in the experiment is the yield.
- The **theoretical yield** is the amount you would get if everything went perfect.
- The **actual yield** is what you make in the lab.

The percent yield

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

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

Learning outcomes

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

Learning outcomes

- **Mole concept and conversions**
- **Empirical and molecular formulas**
 - **Combustion analysis**
- **Stoichiometry**
- **Limiting reactant**
- **% yield**