Chapter 3

Stoichiometry

Atomic Masses

- 1 atomic mass unit (amu) = 1/12 of the mass of a ^{12}C atom so one ^{12}C atom has a mass of 12 amu (exact number).
- From mass spectrometry: $^{13}C/ ^{12}C$ = 1.0836129 amu
- So the mass of a ^{13}C atom is (1.0836129)(12 amu) = 13.003355 amu
- 1 amu = $1.66053873 \times 10^{-27}$ kg
- So the mass of a ^{13}C atom is:

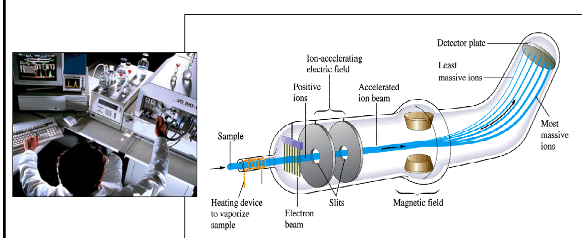
(13.003355 amu)($1.66053873 \times 10^{-27}$kg/amu)

= $2.1592575 \times 10^{-26}$ kg

Chemical Stoichiometry

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

Figure 3.1: (left) A scientist injecting a sample into a mass spectrometer. (right) Schematic diagram of a mass spectrometer.



Mass and Moles of a Substance

- Chemistry requires a method for determining the numbers of molecules in a given mass of a substance.
  - This allows the chemist to carry out "recipes" for compounds based on the relative numbers of atoms involved.
  - The calculation involving the quantities of reactants and products in a chemical equation is called **stoichiometry**.

Average Atomic Mass

·Elements occur in nature as mixtures of isotopes

·We will call the average atomic mass the

·atomic weight

· Atomic weight is based on the

relative abundance of isotopes

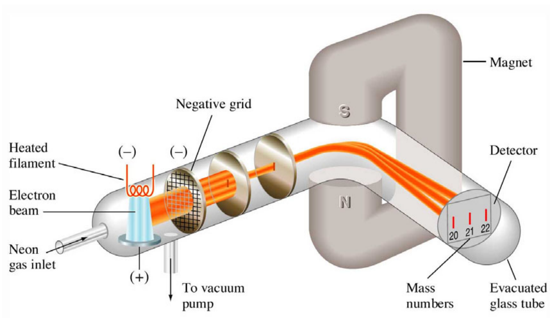
Carbon = 98.89% ^{12}C = 0.9889 x 12 amu = 11.87

1.11% ^{13}C = 0.0111 x 13.003 amu = 0.144

<0.01% ^{14}C = neglect

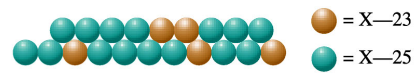
Average carbon atomic weight = 12.01 amu

Figure 2.11: Diagram of a simple mass spectrometer.



Conceptual Problem 2.47: Green and brown spheres.

2.47 While traveling to a distant universe, you discover the hypothetical element, "X." You obtain a representative sample of the element and discover that it is made up of two isotopes, X-23 and X-25. To help your science team calculate the atomic mass of the substance, you send the following drawing of your sample with your report.



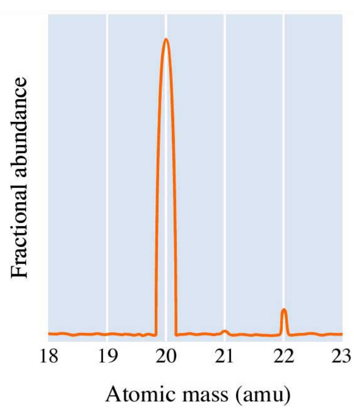
In the report, you also inform the science team that the gold atoms are X-23, which have an isotopic mass of 23.02 amu, and the green atoms are X-25, which have an isotopic mass of 25.147 amu. What is the atomic mass of element X?

Figure 2.12: The mass spectrum of neon.

^{20}Ne = .907

^{21}Ne = .003

^{22}Ne = .090



X-23: (5/20) x 23.02 amu = 5.755

X-25: (15/20) x 25.147 amu = <u>18.860</u>

24.615

Average atomic weight = 24.615 amu

Atomic Weight of Elements

Calculate the average atomic weight of boron, B, from the following data:

ISOTOPE	ISOTOPIC MASS (amu)	FRACTIONAL ABUNDANCE
B-10	10.013	0.1978
B-11	11.009	0.8022

B-10: 10.013 x 0.1978 = 1.9806

B-11: 11.009 x 0.8022 = <u>8.8314</u>

10.8120 = 10.812 amu

The Mole

- One mole is the number equal to the number of carbon atoms in exactly 12 grams of pure ^{12}C.
- The number = $6.02214199 \times 10^{23}$
- 1 mole of anything = 6.022×10^{23} units

Avogadro's number equals

6.022×10^{23} units

Figure 3.2: One mole each of various substances. Photo courtesy of American Color.

Molar Mass

- A substance's molar mass (or molecular weight) is the mass in grams of one mole of the compound.
  - CO_2 = 44.01 grams per mole

		g/mole
1 C	=	12.01
2 O	2 x 16.00 =	32.00
		44.01 g/mole

Determining the Moles of Atoms

How many moles of Se atoms are in 20.0 g of Se?

$$20.0 \text{ g Se} \times \frac{1 \text{ mol Se}}{78.96 \text{ g Se}} = 0.253 \text{ mol Se atoms}$$

← molar mass of Se

How many atoms of Se are in 20.0 g of Se?

$$0.253 \text{ mol Se atoms} \times \frac{6.022 \times 10^{23} \text{ Se atoms}}{\text{mol Se atoms}} = 1.53 \times 10^{23} \text{ Se atoms}$$

TABLE 3.1 Comparison of 1 Mole Samples of Various Elements

Element	Number of Atoms Present	Mass of Sample (g)
Aluminum	6.022×10^{23}	26.98
Copper	6.022×10^{23}	63.55
Iron	6.022×10^{23}	55.85
Sulfur	6.022×10^{23}	32.07
Iodine	6.022×10^{23}	126.9
Mercury	6.022×10^{23}	200.6

Write the molecular formula and calculate the formula weight for hydrogen peroxide and nitric acid

a) H_2O_2

2 x at. wgt. H =	2.02 amu
2 x at. wgt. O =	32.00 amu
	34.02 amu

b) HNO_3

1 x at. wgt. H =	1.01 amu
1 x at. wgt. N =	14.01 amu
3 x at. wgt. O =	48.00 amu
	63.02 amu

Determining Molar Mass

What is the molar mass of $Al_2(SO_4)_3$?

$$1 \text{ mol } Al_2(SO_4)_3 \times \frac{2 \text{ mol Al}}{\text{mol } Al_2(SO_4)_3} \times \frac{26.98 \text{ g}}{\text{mol Al}} = 53.96 \text{ g}$$

$$1 \text{ mol } Al_2(SO_4)_3 \times \frac{3 \text{ mol S}}{\text{mol } Al_2(SO_4)_3} \times \frac{32.07 \text{ g}}{\text{mol S}} = 96.21 \text{ g}$$

$$1 \text{ mol } Al_2(SO_4)_3 \times \frac{12 \text{ mol O}}{\text{mol } Al_2(SO_4)_3} \times \frac{16.00 \text{ g}}{\text{mol O}} = \underline{192.00 \text{ g}}$$

Molar mass of $Al_2(SO_4)_3$ = 342.17 g
= 342.2 g

Figure 3.7:
A welder welding using an oxy-acetylene torch.
Photo courtesy of PhotoDisc.

CH

acetylene

Percent Composition

- Mass percent of an element:

$$\text{mass \%} = \frac{\text{mass of element in compound}}{\text{mass of compound}} \times 100\%$$

- For iron in iron (III) oxide, (Fe_2O_3)

Molar mass of Fe_2O_3 = 159.69 g

Mass of Fe = $1 \text{ mol } Fe_2O_3 \times \frac{2 \text{ mol Fe}}{\text{mol } Fe_2O_3} \times 55.85 \text{ g Fe} = 111.7 \text{ g}$

$$mass \text{ \% } Fe = \frac{111.7}{159.69} \times 100\% = 69.95\%$$

Figure 3.7: Photo of benzene in lab glassware.
Photo courtesy of American Color.

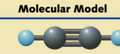
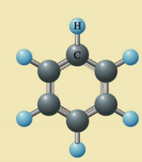
CH

benzene

Determining Chemical Formulas

- Determining the formula of a compound from the percent composition.
  - The percent composition of a compound leads directly to its empirical formula.
  - An **empirical formula** (or simplest formula) for a compound is the formula of the substance written with the smallest integer (whole number) subscripts.

Table 3.1
Molecular Models of Two Compounds That Have the Empirical Formula CH.
Although benzene and acetylene have the same empirical formula, they do not have the same molecular formula or structure.

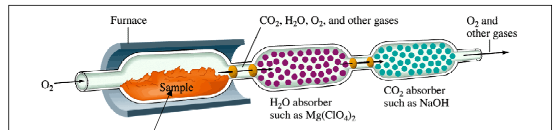
Compound	Empirical Formula	Molecular Formula	Molecular Model
Acetylene	CH	C_2H_2	
Benzene	CH	C_6H_6	

Formulas

- molecular formula = (empirical formula)$_n$
  - [n = integer]
- molecular formula = C_6H_6 = $(CH)_6$ (benzene)
- molecular formula = C_2H_2 = $(CH)_2$ (acetylene)
- empirical formula = CH

Another example: hydrogen peroxide OH = empirical formula
H_2O_2 = molecular formula

Figure 3.5: A schematic diagram of the combustion device used to analyze substances for carbon and hydrogen.



Determining Chemical Formulas

- Determining the empirical formula from the percent composition.
  - Benzoic acid is a white, crystalline powder used as a food preservative. The compound contains 68.8% C, 5.0% H, and 26.2% O by mass. What is its empirical formula?
  - In other words, give the smallest whole-number ratio of the subscripts in the formula

$$C_xH_yO_z$$

Benzoic Acid is a white, crystalline powder used as a food preservative which is 68.8% C, 5.00 % H, and 26.2% O by mass. What is its empirical formula?
For 100.0 g of benzoic acid:

$$68.8 \text{ g C} \times \frac{1 \text{ mol C}}{12.0 \text{ g C}} = 5.73 \text{ mol C}$$

$$5.00 \text{ g H} \times \frac{1 \text{mol H}}{1.01 \text{ g H}} = 4.95 \text{ mole H}$$

$$26.2 \text{ g O} \times \frac{1 \text{ mol O}}{16.0 \text{ g O}} = 1.638 \text{ mol O}$$

divide by 1.638, then empirical formula is $C_{3.5}H_{3.0}O$ or $C_7H_6O_2$

Determining Chemical Formulas

- Determining the empirical formula from the percent composition.
  - For the purposes of this calculation, we will assume we have 100.0 grams of benzoic acid.
  - Then the mass of each element equals the numerical value of the percentage.
  - Since x, y, and z in our formula represent mole-mole ratios, we must first convert these masses to moles.

$$C_xH_yO_z$$

Empirical Formula Determination (when you are given mass percentages of elements)

- 1. Base calculation on 100 grams of compound.
- 2. Determine moles of each element in 100 grams of compound.
- 3. Divide each value of moles by the smallest of the values.
- 4. Multiply each number by an integer to obtain all whole numbers.

Another type of empirical formula problem….

1.0003 g of a compound containing only C, H and O are combusted to form CO_2 and H_2O. If 2.5224 g of CO_2 and 0.4457 g of H_2O are formed, what is the empirical formula of the compound?

1. Calculate the masses of C and H formed:
   2.5224 g CO_2 x (1 mol CO_2/44.01 g CO_2)x(1 mol C/mol CO_2)) x (12.01 g C/mol C) = 0.6883 g C
   0.4457 g H_2O x (1 mol H_2O/18.01 g) x (2 mol H/mol H_2O) x (1.008 g H/mole H) = 0.04990 g H

2. Determine the mass of O by subtracting the masses of C and H from the mass of the compound reacted:
   1.0003 g – (0.6883 g C + 0.04990 g O) = 0.2621 g O

Determining Chemical Formulas

- Determining the molecular formula from the empirical formula.
  – For example, suppose the empirical formula of a compound is CH_2O and its molar mass is 60.0 g/mol.
  – The molar mass of the empirical formula (the empirical weight) is only 30.0 g/mol.
  – This would imply that the molecular formula is actually the empirical formula doubled, or

$(CH_2O)_2 = C_2H_4O_2$

Empirical formula calculation continued….

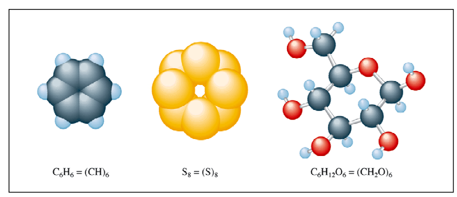
3. Now calculate the moles of C, H and O in the compound:

   moles of C = 0.6883 g C x (1 mol C/12.01 g) = 0.05730 mol C
   moles of H = 0.04990 g H x (1 mol H/1.008 g)= 0.04950 mol H
   moles of O = 0.2621 g O x (1 mol O/16.00 g) = 0.01638 mol O

4. Now divide mol C & mol H by mol O to get ratio of mol C and H to O since it is present in smallest no. moles.
   $\frac{0.05730}{0.01638} = 3.5$ $\frac{0.04950}{0.01638} = 3.0$
   and substitute the coefficients into $C_x H_yO_z$

   to give $C_{3.5}H_3O$ or C_7H_6O - the same empirical formula as benzoic acid!

Figure 3.6: Examples of substances whose empirical and molecular formulas differ. Notice that molecular formula = (empirical formula)$_n$, where *n* is an integer.



Determining Chemical Formulas

- Determining the **molecular formula** from the empirical formula.
  – An empirical formula gives only the smallest whole-number ratio of atoms in a formula.
  – The **molecular formula** should be a multiple of the empirical formula (since both have the same percent composition).
  – To determine the molecular formula, we must know the **molar mass** of the compound.

Chemical Equations

Chemical change involves a reorganization of the atoms in one or more substances.

Chemical Equation

- A representation of a chemical reaction:
- $C_2H_5OH(g) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(g)$

reactants products

1 mole C_2H_5OH + 3 moles O_2 ➜ 2 moles CO_2 + 3 moles H_2O

1 molecule C_2H_5OH + 3 molecules O_2 ➜
2 molecules CO_2 + 3 molecules H_2O

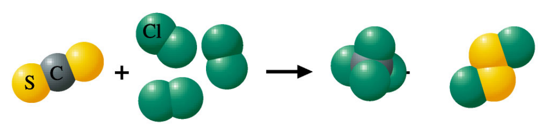
Figure 3.11: Steps in a stoichiometric calculation.

Grams of A × Conversion factor: g A to mol A × Conversion factor: mol A to mol B × Conversion factor: mol B to g B → Grams of B

TABLE 3.2 Information Conveyed by the Balanced Equation for the Combustion of Methane

Reactants		Products
$CH_4(g) + 2O_2(g)$	⟶	$CO_2(g) + 2H_2O(g)$
1 molecule + 2 molecules	⟶	1 molecule + 2 molecules
1 mole + 2 moles	⟶	1 mole + 2 moles
6.022×10^{23} molecules + 2 (6.022×10^{23} molecules)	⟶	6.022×10^{23} molecules + 2 (6.022×10^{23} molecules)
16 g + 2 (32 g)		44 g + 2 (18 g)
80 g reactants	⟶	80 g products

3.79 The following reaction, depicted using molecular models, is used to make carbon tetrachloride, CCl_4, a solvent and starting material for the manufacture of fluorocarbon refrigerants and aerosol propellants.



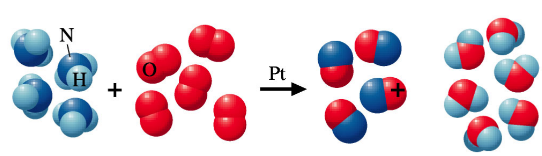
Calculate the number of grams of carbon disulfide, CS_2, needed for a laboratory-scale reaction with 62.7 g of chlorine, Cl_2.

Calculating Masses of Reactants and Products

- 1. Balance the equation.
- 2. Convert mass to moles.
- 3. Set up mole ratios.
- 4. Use mole ratios to calculate moles of desired substituent.
- 5. Convert moles to grams, if necessary.

3.80 Using the following reaction (depicted using molecular models), large quantities of ammonia are burned in the presence of a platinum catalyst to give nitric oxide, as the first step in the preparation of nitric acid.

Suppose a vessel contains 12.2 g of NH_3, how many grams of O_2 are needed for a complete reaction?



CONCEPT CHECK 3.4

The main reaction of a charcoal grill is $C(s) + O_2(g) \longrightarrow CO_2(g)$. Which of the statements below are incorrect? Why?

a. 1 atom of carbon reacts with 1 molecule of oxygen to produce 1 molecule of CO_2.

b. 1 g of C reacts with 1 g of O_2 to produce 2 grams of CO_2.

c. 1 g of C reacts with 0.5 g of O_2 to produce 1 g of CO_2.

d. 12 g of C reacts with 32 g of O_2 to produce 44 g of CO_2.

e. 1 mol of C reacts with 1 mol of O_2 to produce 1 mol of CO_2.

f. 1 mol of C reacts with 0.5 mol of O_2 to produce 1 mol of CO_2.

g. h.

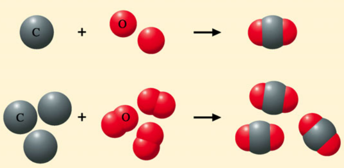
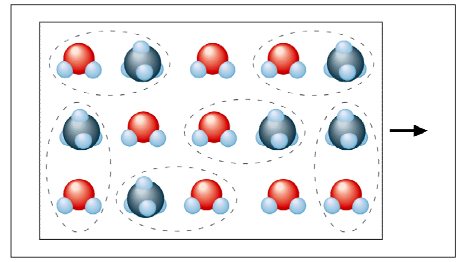


Figure 3.10: A mixture of CH_4 and H_2O molecules.



Limiting Reactant

The limiting reactant is the reactant that is consumed first, limiting the amounts of products formed.

Figure 3.11: Methane and water have reacted to form products according to the equation

$CH_4 + H_2O \rightarrow 3H_2 + CO$.

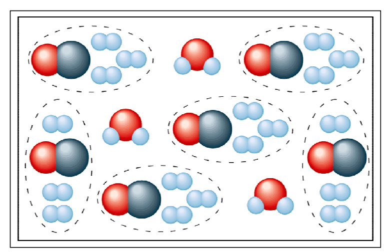


Figure 3.9: Three different stoichiometric mixtures of methane and water, which react one-to-one.

$\mathbf{CH_4 + H_2O \rightarrow 3H_2 + CO}$.

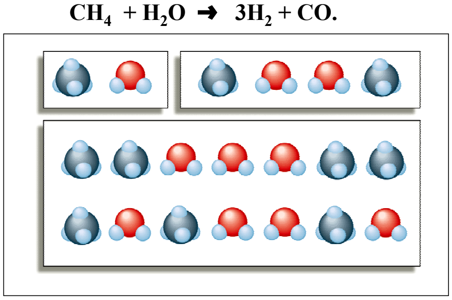
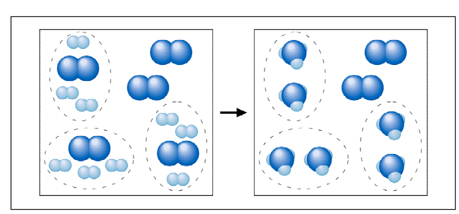


Figure 3.12: Hydrogen and nitrogen react to form ammonia according to the equation

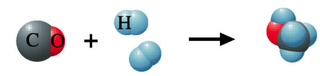
$N_2 + 3H_2 \rightarrow 2NH_3$.



Solving a Stoichiometry Problem

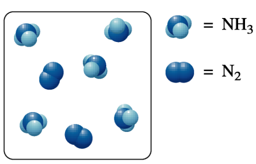
- 1. Balance the equation.
- 2. Convert masses to moles.
- 3. Determine which reactant is limiting.
- 4. Use moles of limiting reactant and mole ratios to find moles of desired product.
- 5. Convert from moles to grams.

3.85 Methanol, CH_3OH, is prepared industrially from the gas-phase catalytic balanced reaction that has been depicted here using molecular models.



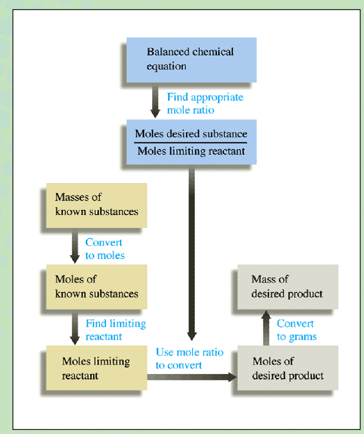
In a laboratory test, a reaction vessel was filled with 35.4 g CO and 10.2 g H_2. How many grams of methanol would be produced in a complete reaction? Which reactant remains unconsumed at the end of the reaction? How many grams of it remain?

3.13 You react nitrogen and hydrogen in a container to produce ammonia, $NH_3(g)$. The following figure depicts the contents of the container after the reaction is complete.

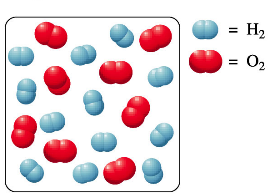


a. Write a balanced chemical equation for the reaction.
b. What is the limiting reactant?
c. How many molecules of the limiting reactant would you need to add to the container in order to have a complete reaction (convert all reactants to products)?

Solving stoichiometry problems flow chart.



3.18 A few hydrogen and oxygen molecules are introduced into a container in the quantities depicted in the following drawing. The gases are then ignited by a spark causing them to react and form H_2O.



a. What is the maximum number of water molecules that can be formed in the chemical reaction?
b. Draw a molecular level representation of the container's contents after the chemical reaction.

Calculating Percent Yield

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

What is the percent yield of menthol if the theoretical yield is 30.0 g and the actual yield is 20.0 g?

$$\frac{20.0\text{ g}}{30.0\text{ g}} \times 100\% = 66.7\%$$