Chapter 3

Stoichiometry

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Introduction

- In this chapter we will consider the quantities of materials consumed and produced in chemical reactions.
- This area of study is called chemical stoichiometry.

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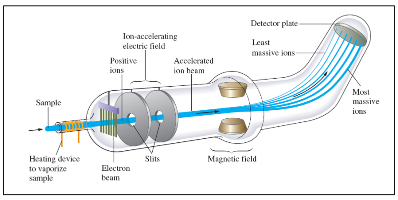
Atomic Masses

- The modern system of atomic masses is based on ^{12}C. In this system ^{12}C assigned a mass of exactly 12 atomic mass units (amu).
- The most accurate method currently available for comparing the masses of atoms involves the use of the mass spectrometer.



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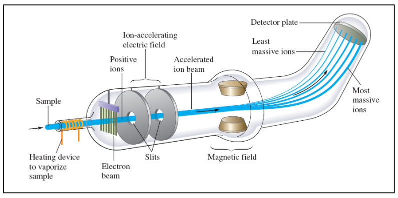
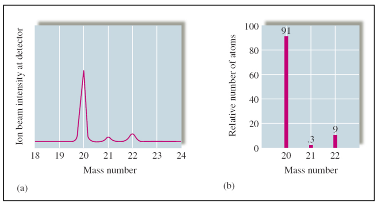
Atomic Masses

- In this instrument, atoms or molecules are passed into a beam of high speed electrons. The high speed electrons knock electrons off the atoms or molecules being analyzed and change them to positive ions.
- The amount of path deflection for each depends on its mass - the most massive ions are deflected the smallest amount - which causes the ions to separate.



Atomic Masses

- Most elements occur in nature as mixture of isotopes; thus atomic masses are usually average values .
- Natural carbon is composed of 98.89% ^{12}C atoms and 1.11% ^{13}C atoms. The amount of ^{14}C is negligibly small.
- The relative intensities of the signals recorded when natural neon is injected into a mass spectrometer.



Mass Spectrum of Neon

Atomic Masses

- This average mass is often called the atomic weight of carbon.
- Eventhough natural carbon does not contain a single atom with mass 12.01, for stoichiometric purposes we consider carbon to be composed of one type of atom with a mass of 12.01 .
- The mass listed for hydrogen (1.008) is the average mass for natural hydrogen, which is a mixture of ^{1}H and ^{2}H (deuterium)

Atomic Masses

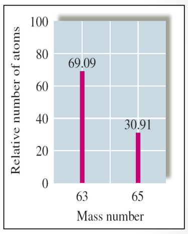
- Example 3.1:

To find the average masses of natural copper, ^{63}Cu (62.93 amu) and ^{64}Cu (64.93 amu):

For every 100 atoms, we have on average 69.09 atoms of ^{63}Cu and 30.91 atoms of ^{64}Cu. Thus the average mass of 100 atoms of natural copper is:

$62.93 \times 69.09 + 64.93 \times 30.91 =$
6355 amu / 100 atoms

So in one copper atom, the average mass is 63.55 amu



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Atomic Masses

- The element magnesium (Mg) has three stable isotopes with the following masses and abundances. Calculate the atomic mass of magnesium.

Isotope	Mass (amu)	Abundance
^{24}Mg	23.9850	78.99%
^{25}Mg	24.9858	10.00%
^{26}Mg	25.9826	11.01%

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The Mole

- The mole (abbreviated mol) is the number equal to the number of carbon atoms in exactly 12 grams of ^{12}C.
- Avogadro's number is: 6.022137×10^{23} (6.022×10^{23})
- One mole of something consists of 6.022×10^{23} units of that substance.
- 1 mol can be described as:
  - 6.022×10^{23} **atoms** so we use "Atomic mass of an element
  - 6.022×10^{23} **molecules** so we use " Molecular weight (M.w) of molecule"

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The Mole

- Example 3.2: Find the mass of 6 atoms of Americium.

Note that one americium atom has a mass of 243 amu.

Note that this atom does not occur naturally, It could be made in a device called particle accelerator

We know that each 243 grams of this atom contains 6.022×10^{23} atoms, so 6 atoms must weigh:

$6 \times 243 / 6.022 \times 1023 = 2.42 \times 10^{-21}$g

Note: n moles → N_A molecules

*Do example 3.3 (H.W)

Molar Mass

- The mass, in grams, of 1 mol of a substance is termed as "Molar mass"
- The term molecular weight has been used to describe the mass of 1 mole of a substance. Thus terms molar mass and molecular weight mean exactly the same thing: the **mass** in **grams** of 1 **mole** of a compound.
- Some substances exist as a collection of ions rather than as separate molecules. For example in some texts the term formula weight is used for ionic compounds.

Molar Mass

Ex 3.4: How many molecules of isopentyl acetate ($C_7H_{14}O_2$) are present in 1 µg? The is the amount of isopentyl acetate released by a bee when it stings. How many atoms of carbon are present?

x molecules ⟶ 1×10^{-6} g

6.02×10^{23} molecules ⟶ 130 g

1 molecule ⟶ 7 atoms C

5×10^{15} molecules ⟶ X atoms C

Molar Mass

Example 3.4:
Isopentyl acetate $C_7H_{14}O_2$ of mass 1×10^{-6} g :

Mass of 1 mol of $C_7H_{14}O_2$ = 7 mol C × 12.011 + 14 mol H × 1.0079 + 2 mol O × 15.999 = 130.186 g

- In 6.022×10^{23} molecules (1 mol) we have 130.186 g of the compound, thus in 1×10^{-6} g, we have:

$$\frac{1 \times 10^{-6} \times 6.022 \times 10^{23}}{130.186} = 5 \times 10^{15} \text{ molecules}$$

- In 1 molecule of the compound we have 7 molecules of Carbon, so in 5×10^{15} molecules we have of the compound, we have:

$$\frac{5 \times 10^{15} \times 7}{1} = 4 \times 10^{16} \text{ atoms of carbon}$$

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Percent Composition of Compounds

Consider ethanol C_2H_5OH
- Mass of C = 2 mol × 12.011 g/mol = 24.022 grams
- Mass of H = 6 mol × 1.008 g/mol = 6.048 grams
- Mass of O = 1 mol × 15.999 g/mol = 15.999 grams
- Mass of 1 mol of C_2H_5OH = 46.069g

The mass percent of carbon in ethanol can be computed by comparing the mass of carbon in 1 mole of ethanol:

$$\text{Mass percent of C} = \frac{\text{mas of 1 mol C}}{\text{M.w of compound}} \times 100\%$$

- % of C = × 100 % = 52.144 %
- % of H = × 100 % = 13.13 %
- % of O = × 100 % = 34.728 %

*Do example 3.5 (H.W)

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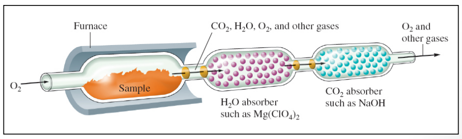
Formula Determination

- The formula is determined by taking a weighed sample of the compound and either decomposing it into its component elements or reacting it with oxygen to produce substances such as CO_2, H_2O & N_2 which are then collected and weighed.
- The results of such analyses provide the mass of each type of element in the compound, which can be used to determine the mass percent of each element present.



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Formula Determination

- **Empirical formula** is the simplest whole-number ratio of the various types of atoms in a compound
- **Molecular formula** is the *exact* formula of a molecule and can be determined if we also know the molar mass
- E.g. A compound with the empirical formula CH_5N could have a molecular formula of CH_5N, $C_2H_{10}N_2$ or $C_3H_{15}N_3$ or $C_4H_{20}N_4$ …
- Any molecule that can be represented as $(CH_5N)_x$ where *x* is an integer has the empirical formula CH_5N

Molecular formula = (empirical formula)$_x$ where *x* is an integer

Determining the Formula of a Compound

Suppose a substance has been prepared that is composed of carbon, hydrogen and nitrogen.

- When 0.1156 gram of this pound is reacted with oxygen, 0.1638 gram of carbon dioxide (CO_2) and 0.1676 gram of water (H_2O) are collected.
- Assuming that all of carbon in the compound is converted to CO_2, we can determine the mass of carbon originally present in the 0.1156 gram sample.
- To do so, we must use the percentage by mass of carbon in CO_2. The molar mass of CO_2 is 12.011 g/mol + 2(15.999 g/ mol) = 44.009 g /mol.
- The fraction of carbon present (12.011 grams C per 44.009 grams CO_2) can now be used to determine mass of carbon in 0.1638 gram of CO_2**:**

0.1638 g CO_2 × 12.011 / 44.009 g CO_2 = 0.04470 g C , which represents 38.67 % by mass of the compound.

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Determining the Formula of a Compound

- Similarly for H:

0.1676 g H_2O × 2.016 g H / 18.015 g H_2O = 0.01876 g H, which represent

16.23 % by mass of the compound

Since the unknown compound contains only C, H and N:

% N = 100 – (38.67 % + 16.23 %) = 45.10 % N

- To determine the formula of the compound:

In 100 grams of the compound, we have 38.67 g C, 16.23 g H and 45.10 g N:

n (C) = 38.67 / 12.011 = 3.220 mol C

n (H) = 16.23 / 1.008 = 16.10 mol H

n (N) = 45.10 / 14.007 = 3.220 mol N

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Determining the Formula of a Compound

Find the smallest whole-number ratio of atoms:

C: $\frac{3.220}{3.220} = 1$

H: $\frac{16.10}{3.220} = 5$

N: $\frac{3.220}{3.220} = 1$

- The formula is thus CH_5N .
- This formula is called the **empirical formula.**

Determining the Formula of a Compound

- Example 3.6: Compound with 43.64% phosphorus and 56.36% oxygen by mass (Molar Mass = 283.88 g).

To find the empirical and molecular formulas:

- In 100 g of the compound, we find: n = mass / M.w
  43.64/31 = 1.4 mol P and 56.36 / 16 = 3.5 mol O
  Then: 1.4/1.4 = **1** for P and 3.5 /1.4 = **2.5** for O
- Multiply both by 2: we get P_2O_5 which is the "empirical" formula

M.w = 2 × 31 + 16 ×5 = 141.9 g/mol

$(P_2O_5)x$ = 283.88 g/mol so (141.9).x = 283.88, we get x = 2 so $(P_2O_5)_2$

Therefore the molecular formula is P_4O_{10}

*Do example 3.7 (H.W)

Example 3.6

P_xO_y ; M.w. = 283.88 g/mol

In 100 g:

P: 43.64% ; 43.64 g /31 = 1.4 /1.4 = 1 x 2 = 2

O: 56.36% ; 56.36 g / 16 = 3.5/1.4 = 2.5 x 2 = 5

P_2O_5 is E.F. and M.w. = 141.9 g/mol

(141.9)x = 283.88

x = 2

M.F is P_4O_{10}

Determining the Formula of a Compound

➢To Determine the Empirical Formula:

- Base the calculation on 100 grams of the compound. Each mass percent will represent the mass in grams of that element present in the compound.
- Determine the number of moles of the each element present in 100 grams of that compound using atomic weights
- Divide each value of the number of moles by the smallest value. If each resulting number is a whole number, they represent the subscripts of the elements in empirical formula.
- If the numbers are not whole numbers, multiply each by an integer so that the results are whole numbers.

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Determining the Formula of a Compound

➢To Determine the Molecular Formula:

- Obtain empirical formula .
- Compute the empirical formula mass
- Calculate the ratio
  MOLAR MASS / EMPIRICAL FORMULA MASS
- The integer from the previous step represents the number of empirical formula units in one molecule .
- When the empirical formula subscripts are multiplied by this integer, we obtain the molecular formula .

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Chemical Equations

➢A chemical change involves reorganization of the atoms .

When the methane (CH_4) in natural gas combines with oxygen (O_2) in the air and burns, carbon dioxide (CO_2) and water (H_2O) are formed. The process is represented by a chemical equation with the reactants on the left side of an arrow and products on the right side.

$$\underbrace{CH_4 + O_2}_{\text{REACTANTS}} \rightarrow \underbrace{CO_2 + H_2O}_{\text{PRODUCTS}}$$

➢Bonds have been broken and new ones have been formed. In a chemical reaction atoms are neither created nor destroyed. All atoms present in the reactants must be accounted for among the products .

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Chemical Equations

- Balancing chemical equation : $CH_4 + 2O_2 \rightarrow CO_2 + 2 H_2O$
- The chemical equation of a reaction provides 2 important types of information:
  - The nature of reactants and products and the relative number of each.
- The equation often includes the physical state of the reactants and products.

State	Symbol
Solid	(s)
Liquid	(l)
Gas	(g)
Dissolved in water (in aqueous solution)	(aq)

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Chemical Equations

- Example:

$HCl\ (aq) + NaHCO_3\ (s) \rightarrow CO_2\ (g) + H_2O\ (l) + NaCl\ (aq)$

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

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

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Balancing Chemical Equations

- Atoms are conserved in a chemical reaction.
- The formulas of the compounds must never be changed when balancing a chemical equation.
- In balancing equations, start with the most complicated molecule
  - Example:

    $C_2H_5OH\ (l) + O_2(g) \rightarrow CO_2(g) + H_2O\ (g)$

  - The most complicated molecule here is C_2H_5OH.
  - The balanced equation becomes:

$C_2H_5OH\ (l) + 3O_2(g)$ ---> $2CO_2(g) + 3H_2O\ (g)$

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Balancing Chemical Equations

- STEPS : Writing and Balancing the Equation for a Chemical Reaction
  - Determine what reaction is occurring . What are the reactants , the products, and the states involved ?
  - Write the unbalanced equation that summarizes the preceding information .
  - Balance the equation by inspection , starting with the most complicated molecule(s) .
  - Determine what coefficients are necessary to ensure that the same number of each type of atoms appears on both reactants and products sides . Do not change the identities (formulas) of any of the reactants or products

*Do Example 3.8 (H.W)

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Stoichiometric Calculations

- **Amounts of Reactants and Products:**
  - Coefficients in chemical equations represent number of molecules.
  - In the laboratory or chemical plant when a reaction is to be run, the amounts of substances needed cannot be determined by counting molecules directly.
- Consider the combustion of propane (C_3H_8):

What mass of oxygen (O_2) and carbon dioxide (CO_2) will react with 96.1 gram of propane?

- Write the balanced chemical equation for the reaction:

$$C_3H_8\,(g) + 5O_2\,(g) \rightarrow 3CO_2\,(g) + 4\,H_2O\,(g)$$

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Stoichiometric Calculations

$C_3H_8\,(g) + 5O_2\,(g) \rightarrow 3CO_2\,(g) + 4\,H_2O\,(g)$

96.1 g/ 44.1 x g / 5×32 y g / 3×44

We get: x = 349 g O_2 and y = 288 g CO_2

Another Method:

- Find the number of moles of propene then that of O_2 ($n_{O2} = m_{O2}$/ M.w)
- We get : 2.18 mol C_3H_8
  10.9 mol O_2
  6.54 mol CO2
- Thus the mass of O_2 = 10.9 × 32.0 = 349 g O_2
- The mass of CO_2 = 288 g O_2

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Stoichiometric Calculations

STEPS : Calculation of Masses of Reactants and Products in Chemical Reactions:

- Balance the equation for the reaction.
- Convert the known masses of substances to moles .
- Use the balanced equation to set up the appropriate mole ratios.
- Use the appropriate mole ratios to calculate the number of moles of the desired reactant or product .
- Convert from moles back to grams if required by the problem.

*Do Example 3.9 (H.W)

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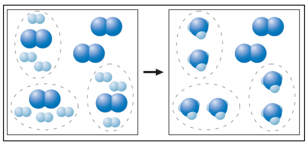
Calculations Involving a Limiting Reactant

- Stoichiometric quantities: exactly the correct amounts so that all reactants "Run Out " (are used up) at the same time.
- HABER PROCESS: N_2 (g) + $3H_2$(g) $\rightarrow 2NH_3$ (g)
- Assume that 5 N_2 molecules and $9H_2$ molecules are placed in a flask. Is this a stoichiometric mixture of reactants, or will one of them be consumed before the other runs out ?



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Calculations Involving a Limiting Reactant

- Write the reaction:

N_2 (g) + $3H_2$(g) $\rightarrow 2NH_3$ (g)

5/1 9/3

5 > 3

excess limiting

Thus, H_2 is the limiting reactant and it's consumed before N_2.

- In any stiochiometry problem it's essential to determine which reactant is the limiting reactant because it, by definition, ***limits the amount of product formed.***
- Establish a mole ratio between limiting reactant and product.

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Calculations Involving a Limiting Reactant

- Suppose 25.0 kilograms of nitrogen & 5.00 kilograms of hydrogen are mixed and reacted to form ammonia. What is the mass of ammonia produced when this reaction is run to completion?

N_2 (g) +	$3H_2$(g) →	$2NH_3$ (g)
25×10^3 g	5×10^3 g	x g
Excess	Limiting	

Therefore hydrogen is the *limiting* reactant in a particular situation , and we must use the amount of hydrogen to compute the quantity of ammonia formed:

Mass (NH_3) = x = $34 \times 5 \times 10^3 / 3 \times 2$ = 28.0 kg NH_3

Another Method:
- Calculate number of moles of N_2
- Calculate the number of moles of required H_2
- Compare

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Calculations Involving a Limiting Reactant

- EXAMPLE 3.10: 18.1 g of ammonia is reacted with 90.4 g of copper(II) oxide. Determine the mass of nitrogen produced.

	$2NH_3$ (g) +	3CuO(s) →	N_2 (g) + 2Cu (s) + $3H_2O$
Masses (g):	18.1 / 2×17	90.4/ 2×79.5	(x)/14×2
	0.532 >	0.379	

So we can find the mass of N_2 :

x = 10.61 g N_2

- The amount of a given product formed when the limiting reactant is completely consumed is called the **theoretical yield** of the product. This maximum amount of nitrogen that can be produced from the quantities of reactants used.

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Calculations Involving a Limiting Reactant

- The actual yield of product is often given as percentage of the theoretical yield. This value is called **percent yield**:

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

- If the reaction considered in example 3.10 actually produced 6.63 gram of nitrogen instead of the predicted 10.6 gram, the percent yield of nitrogen would be

$$\frac{6.63 \text{ g N2}}{10.6 \text{ g N2}} \times 100\% = 62.5\ \%$$

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Solving a Stoichiometry Problem Involving Masses of Reactants and Products

- <u>STEPS</u>
  - Write and balance equation of the reaction.
  - Convert the masses of known substances into moles.
  - By comparing the mole ratio required by the balanced equation with the mole ratio of reactants actually present, determine which reactant is limiting.
  - Using the amount of limiting reactant and the appropriate mole ratios, compute the number of moles of desired product.
  - Convert from moles to grams using molar mass.

*Do Example 3.11 (H.W)

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