

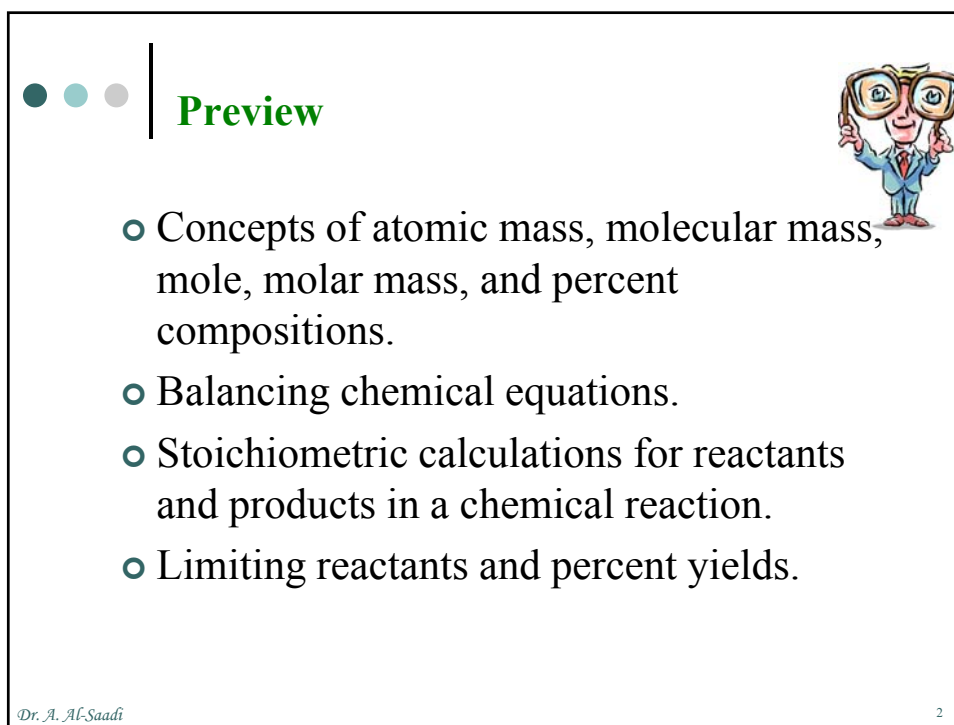
Chapter 3

Stoichiometry

Ratios of Combination

Dr. A. Al-Saadi

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Preview

- Concepts of atomic mass, molecular mass, mole, molar mass, and percent compositions.
- Balancing chemical equations.
- Stoichiometric calculations for reactants and products in a chemical reaction.
- Limiting reactants and percent yields.

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Molecular Mass

- **Molecular Mass** : “some times called molecular weight”; mass of an individual molecule in atomic mass units (amu).
- **Example: Calculate the molecular mass for carbon dioxide, CO₂.**

Write down each element; multiply by atomic mass

$$\text{C} = 1 \times 12.01 = 12.01 \text{ amu}$$

$$\text{O} = 2 \times 16.00 = 32.00 \text{ amu}$$

$$\text{Total mass} = 12.01 + 32.00 = 44.01 \text{ amu}$$

Formula Mass

- **Formula Mass** : mass of the “formula unit” of an ionic compound in atomic mass units (amu) from its *empirical formula*.
- **Example: Calculate the formula mass for barium phosphate.**

Barium phosphate has the empirical formula Ba₃(PO₄)₂

$$\text{Ba} = 3 \times 137.3 = \underline{\hspace{2cm}} \text{ amu}$$

$$\text{P} = 2 \times 30.97 = \underline{\hspace{2cm}} \text{ amu}$$

$$\text{O} = 4 \times 2 \times 16.00 = \underline{\hspace{2cm}} \text{ amu.}$$

$$\text{Total mass} = \underline{\hspace{1cm}} + \underline{\hspace{1cm}} + \underline{\hspace{1cm}} = \underline{\hspace{2cm}} \text{ amu}$$

Percent Composition of Compounds

- Mass % can be calculated by comparing the molecular mass of the atom to the molecular mass of the molecule.
- % composition allows verification of purity of a sample

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

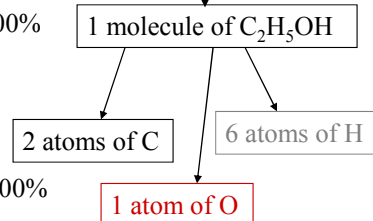
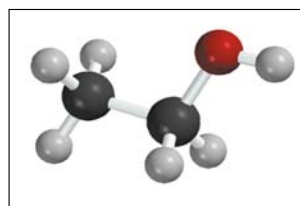
Percent Composition of Compounds

- Mass % can be calculated by comparing the molecular mass of the atom to the molecular mass of the molecule.

- **Example: ethanol (C₂H₅OH):**

$$\begin{aligned} \text{Mass \% O} &= \frac{1 \text{ (atomic mass of O)}}{\text{molec. mass of C}_2\text{H}_5\text{OH}} \times 100\% \\ &= (100\%) \frac{16.00 \text{ amu}}{46.07 \text{ amu}} = 34.73\% \end{aligned}$$

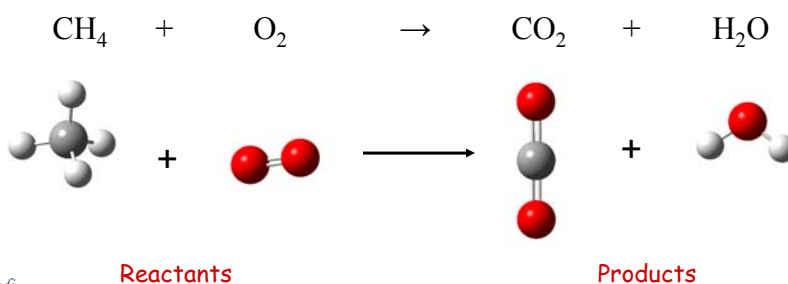
$$\begin{aligned} \text{Mass \% H} &= \frac{6 \text{ (atomic mass of H)}}{\text{molec. mass of C}_2\text{H}_5\text{OH}} \times 100\% \\ &= (100\%) \frac{6(1.01) \text{ amu}}{46.07 \text{ amu}} = 13.13\% \end{aligned}$$



Mass %'s must be added up to 100%

Chemical Equations

- A **chemical reaction** is the chemical change involving *reorganization* of the atoms in one or more substances by *breaking* bonds and *forming* other new bonds.
- This is represented using a **chemical equation**.

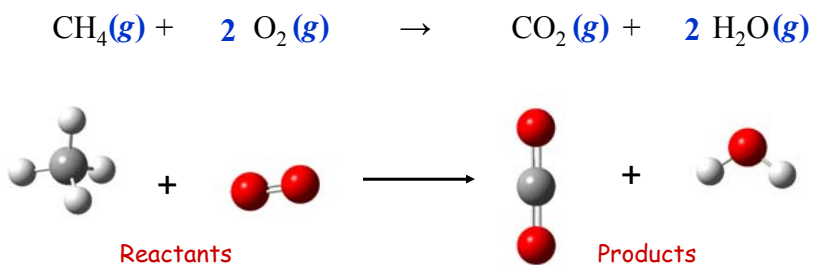


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Chemical Equations

- Chemical equations must be *balanced* so that the numbers of each type of atoms in the reactant and product sides are equal.
- **Physical states** are also indicated in the chemical equation.

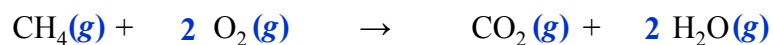


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Chemical Equations

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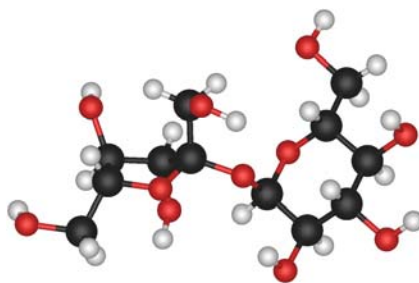
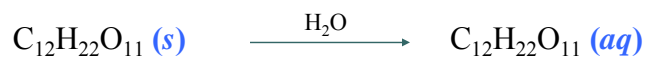


Physical States
of Products and
Reactants



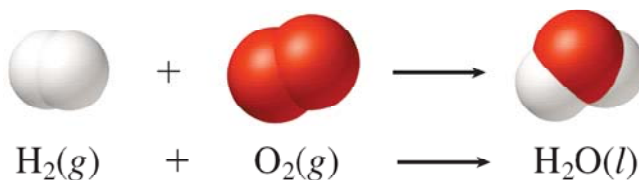
Chemical Equations

- Chemical equations can be also used to describe *physical processes* such as the dissolving of sucrose in water.



Balancing Chemical Equations

- Chemical equations **must be balanced** in order to make sense. Unbalanced equations violate the law of conservation of mass.



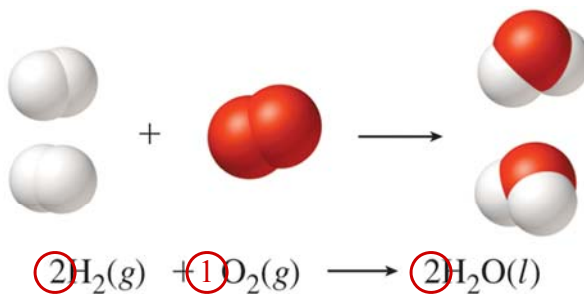
- Balancing achieved by writing appropriate *stoichiometric coefficients* for each reactant and product.

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Balancing Chemical Equations

- Chemical equations **must be balanced** in order to make sense. Unbalanced equations violate the law of conservation of mass.



- Balancing achieved by writing appropriate *stoichiometric coefficients* for each reactant and product.

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Balancing Chemical Equations



- Tips in balancing a chemical equation:
 - You can only change the reaction coefficients, not the atom subscripts or the molecular formulas.
 - Use trial and error methods.
 - Change coefficients for compounds *before* changing coefficients for elements.
 - *Count carefully*, being sure to recount *after each coefficient change*.
 - Write the balanced equation in the final form and do a *reality check*.
 - Train yourself by doing more problems.

Exercises

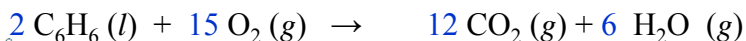
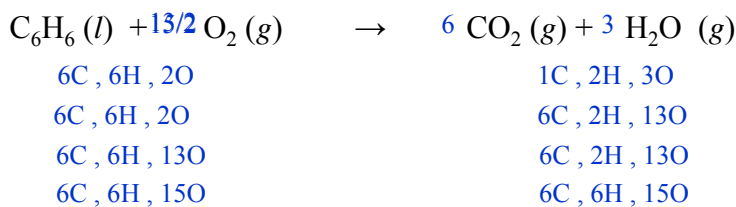
Exercise I



Balancing the hydrogen and oxygen in one step:



Exercise II

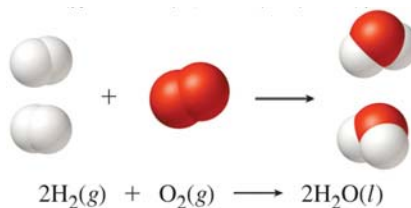


More Exercises



The Concept of the Mole

- Chemists must work with the chemical reactions on a macroscopic level rather than few number of molecules.



- Molecules combine in the ratio specified by the stoichiometric coefficients in the chemical equation.

The Concept of the Mole

- 1 *dozen* of doughnuts contains exactly 12 doughnuts.
- 1 *mole* of a substance contains 6.02214×10^{23} , Avogadro's number (N_A), entities of that substance.

$$6.022 \times 10^{23} = 602,200,000,000,000,000,000,000$$

Can you imagine it??

- 1 mole of seconds
- 1 mole of marbles
- 1 mole of paper sheets

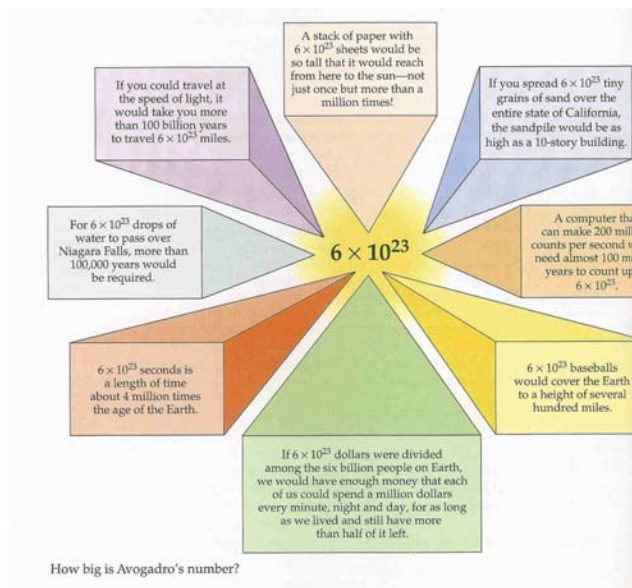
Try this website:

http://www2.ucdsb.on.ca/tiss/stretton/ChemFilm/Mole_Concept/sld001.html

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How Big is the Mole??



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The Moles in Chemistry

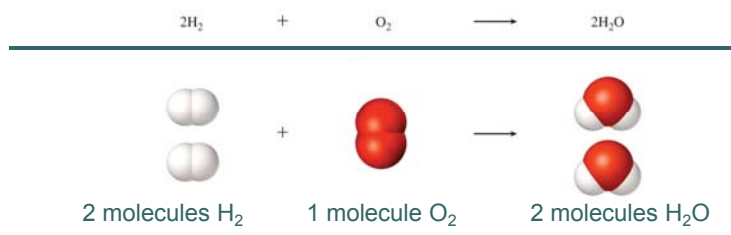
- Scientific (SI) definition of the mole:
 - 1 mole is the number of carbon atoms contained in exactly 12-g sample of pure ^{12}C .
 - The mole is our “counting number” for atoms, molecules and ions much like a dozen is our counting number for cookies or doughnuts.



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The Moles in Chemistry



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Chapter 3 Section 4

The Moles in Chemistry

$$2\text{H}_2 + \text{O}_2 \longrightarrow 2\text{H}_2\text{O}$$

2 molecules H_2 1 molecule O_2 2 molecules H_2O

22.4 L 22.4 L 22.4 L 36 mL

2 moles H_2 1 mole O_2 2 moles H_2O

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Chapter 3 Section 4

The Mole in the Chemical Equation

How much information can balanced chemical reactions give us??

Reaction coefficients Physical state of the compound

Reactants	Products
$1 \text{CH}_4(g) + 2 \text{O}_2(g)$	$1 \text{CO}_2(g) + 2 \text{H}_2\text{O}(g)$
1 molecule + 2 molecules	1 molecule + 2 molecules
1 mole + 2 moles	1 mole + 2 moles
6.022×10^{23} molecules + $2 (6.022 \times 10^{23})$ molecules	6.022×10^{23} molecules + $2 (6.022 \times 10^{23})$ molecules

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Chapter 3 Section 4

Moles and Atoms

Number of moles

Multiply by N_A

Divide by N_A

Number of atoms, molecules, or formula units

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

- Example: Calculate the number of atoms found in 4.50 moles of silicon.
- Example: How many moles of silicon are in 2.45×10^{45} atoms?

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Chapter 3 Section 4

Molar Mass

- Chemists count the number of atoms by measuring their mass.
- **Molar Mass** of a given substance is the mass in grams of 1 mole of that substance.
- By definition, the mass of 1 mole of ^{12}C is exactly 12 g.

For any substance (**numerically**):
Atomic mass (amu) = Mass for 1 mole (g/mol)

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Molar Mass

- 12 g of ^{12}C has 1 mole of ^{12}C atoms. (By definition)
- 12.01 g of C has 1 mole of C atoms.

Because $\frac{12\text{g}}{12.01\text{g}} = \frac{12\text{ amu}}{12.01\text{amu}}$

Relative masses of a single atom of ^{12}C and natural C

Then both samples of ^{12}C and natural C contain the same no. of components (1 mole).

This is applied on all other elements when their masses are determined with respect to the mass of the ^{12}C atom.

Molar Mass

C

Average weight = 12.010 amu
1 mole weighs 12.010 g

He

Average weight = 4.003 amu
1 mole weighs 4.003 g

For any substance (numerically):
Atomic mass (amu) = Mass for 1 mole (g/mol)

Molar Mass

- 1 mole of Li atoms = 6.022×10^{23} Li atoms = 6.941 g of Li.
- Al???
- 1 mole of Al atoms = 6.022×10^{23} Al atoms = 26.98 g of Al.
- Mercury??
- 1 mole of Hg atoms = 6.022×10^{23} Hg atoms = 200.6 g of Hg.

Molar Mass

- **Molar mass** of a compound is obtained by adding up the atomic masses of the atoms composing the compound.
- Examples (MM = molar mass):
 - Atomic mass for O = 16.00 g/mol.
 - Atomic mass for C = 12.01 g/mol.
 - MM for CO = $(12.01 + 16.00)$ g/mol = 28.01 g/mol.
 - MM for CaCO₃ = $(40.08 + 12.01 + 3 \times 16.00)$ g/mol.
= 100.09 g/mol.

Chapter 3 Sections 4

Summary

- Mass of a ^{12}C atom = 12 amu. (by definition)
- Mass of 1 mole of ^{12}C = 12 g
- Mass of 1 mole of element X in grams is **numerically** equal to the average atomic mass of the same element in atomic mass unit (amu).
- 1 mole = 6.022×10^{23} = Avogadro's number
- Molar mass (MM) = the mass of 1 mole of a substance usually expressed in g/mol.

1 1A		2 2A
1 H 1.008		
3 Li 6.941		4 Be 9.012
11 Na 22.99		12 Mg 24.31
19 K 39.10		20 Ca 40.08
37 Rb 85.47		38 Sr 87.62
55 Cs 132.9		56 Ba 137.3
87 Fr (223)		88 Ra (226)

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Chapter 3 Sections 4

Group Activity

16 S 32.06	56 Ba 137.30	25 Mn 54.94
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- The atomic mass of a sulfur atom is amu.
- 1 mol of sulfur has the mass of grams.
- 1 mole of sulfur contains atoms of sulfur atoms.

- The atomic mass of a barium atom is amu.
- 1 mol of barium has the mass of grams.
- 1 mole of barium contains atoms of barium atoms.

- The atomic mass of a manganese atom is amu.
- 1 mol of manganese has the mass of grams.
- 1 mole of manganese contains atoms of manganese atoms.

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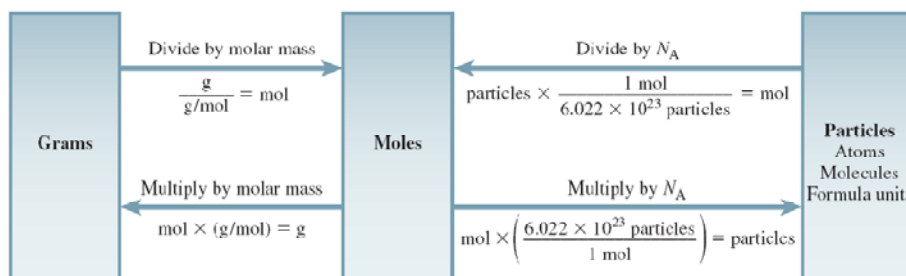
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Moles and Molar Masses

Exercise

- Calculate the molar mass of juglone ($C_{10}H_6O_3$).
- How many moles of juglone are in a $1.56 \times 10^{-2} \text{g}$ sample?

Interconverting mass, moles and number of particles



Moles and Molar Masses

Exercise:

A diamond contains 5.0×10^{21} atoms of carbon. What amount (moles) of carbon and what mass (grams) of carbon are in this diamond?

$$\# \text{ moles of C} = 5.0 \times 10^{21} \text{ atoms of C} \times \frac{1 \text{ mole of C}}{6.022 \times 10^{23} \text{ atoms of C}}$$

$$\text{mass in g} = 5.0 \times 10^{21} \text{ atoms of C} \times \frac{1 \text{ mole of C}}{6.022 \times 10^{23} \text{ atoms of C}} \times \frac{12.01 \text{ g of C}}{1 \text{ mole of C}}$$

Moles and Molar Masses

Exercise:

Molar Mass and Numbers of Molecules

Isopentyl acetate ($C_7H_{14}O_2$) is the compound responsible for the scent of bananas. A molecular model of isopentyl acetate is shown in the margin below. Interestingly, bees release about $1 \mu\text{g}$ (1×10^{-6} g) of this compound when they sting. The resulting scent attracts other bees to join the attack. How many molecules of isopentyl acetate are released in a typical bee sting? How many atoms of carbon are present?

Moles and Molar Masses

What number of atoms of nitrogen are present in 1.00 g of



- MM of $N_2H_4 = (14.01 \times 2 + 1.01 \times 4) \text{ g/mol} = 32.06 \text{ g/mol}$

of N_2H_4 molecules in 1 g of $N_2H_4 =$

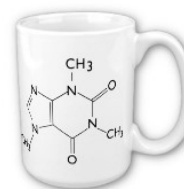
$$1 \text{ g } N_2H_4 \times \frac{1 \text{ mol } N_2H_4}{32.06 \text{ g } N_2H_4} \times \frac{6.022 \times 10^{23} \text{ molec } N_2H_4}{1 \text{ mol } N_2H_4}$$

of N atoms in 1 g of N_2H_4 molecules =

$$\# \text{ of } N_2H_4 \text{ molecules} \times \frac{2 \text{ N atoms}}{1 \text{ molec } N_2H_4}$$

Determining Empirical Formula from Percent Composition

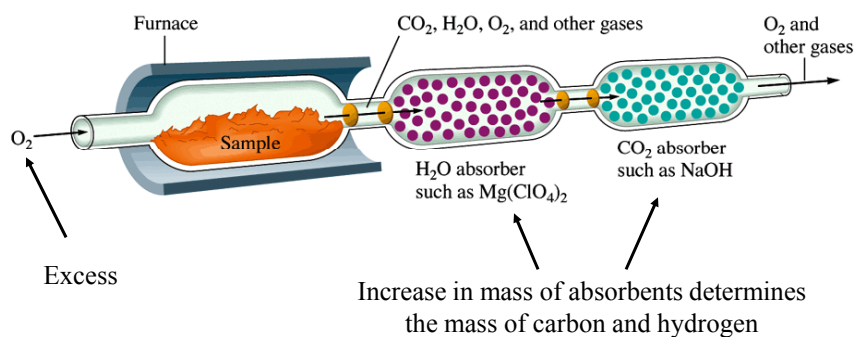
- Empirical formula** : simplest whole-number ratio of atoms in a formula
- Molecular formula** : the “true” ratio of atoms in a formula; often a whole-number multiple of the empirical formula
- We can determine empirical formulas from % composition data; a good analysis tool.



Combustion Analysis

- Combustion of the sample is one of the techniques used to analyze for carbon and hydrogen.

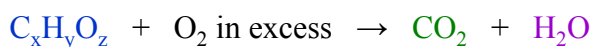
It is done by reacting the sample with O_2 to produce CO_2 , H_2O , and N_2 .



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Determination of the Empirical Formula



Limiting
reactant

Excess

18.8g



27.6g

11.3g

What is the chemical formula of $C_xH_yO_z$??

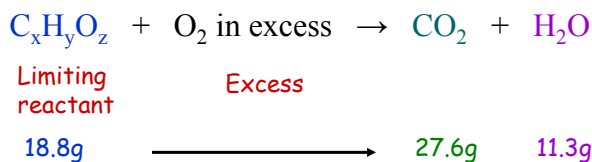
- (a) How much C are in CO_2 = How much C are in $C_xH_yN_z$ \longrightarrow Mass % of C in $C_xH_yN_z$ \longrightarrow Then you do the same thing for H
- (b) Get mass% for O by simple subtraction
- (c) Find # mol of C, H and O per 100g of $C_xH_yO_z$ \longrightarrow (d) Find # the smallest whole number ratio \longrightarrow Empirical formula

Continue \rightarrow

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Determination of the Empirical Formula



What is the empirical formulas of $\text{C}_x\text{H}_y\text{O}_z$??

(a) MM of $\text{CO}_2 = 12.01 + 2(16.00) = 44.01 \text{ g/mol}$

$$\begin{aligned}
 \text{Mass of C in CO}_2 &= 27.6 \text{ g CO}_2 \times \left[\frac{12.01 \text{ g C}}{44.01 \text{ g CO}_2} \right] \\
 &= 7.53 \text{ g C.}
 \end{aligned}$$

Fraction of C
present by
mass in CO_2

$$\text{\% Mass of C in C}_x\text{H}_y\text{O}_z = 7.53 \text{ g C} / 18.8 \text{ g C}_x\text{H}_y\text{O}_z \times 100\% = 40.1\% \text{ C}$$

Continue →

Determination of the Empirical Formula

Similarly:

$$\text{Mass of H in H}_2\text{O} \rightarrow \text{\% Mass of H in C}_x\text{H}_y\text{O}_z \rightarrow 6.74\% \text{ H}$$

(b) Then:

$$100\% - \text{\% mass C} - \text{\% mass H} = \text{\% mass O} = 53.2\% \text{ O}$$

(c) Assuming having 100 g of $\text{C}_x\text{H}_y\text{O}_z$, there will be 40.1g C, 6.74g H, and 53.2g O.

$$\# \text{ mol of C} = 40.1 \text{ g C} \times \left[\frac{1 \text{ mol C}}{12.01 \text{ g C}} \right] = 3.34 \text{ mol C}$$

In the same way: we get 6.67 mol H and 3.33 mol O.

(d) Finding the smallest whole number ratio by dividing by 3.2:

$$\text{C} \rightarrow 1.0 \quad \text{H} \rightarrow 2.0 \quad \text{O} \rightarrow 1.0$$

The (empirical) formula is $\text{C}_1\text{H}_2\text{O}_1$ or simply CH_2O

Determination of the Molecular Formula

The **molecular mass** is needed to determine the molecular (actual) formula.

If MM = 30.03 then it is CH₂O

If MM = 60.06 then it is C₂H₄O₂

and so on...

If C_xH_yO_z is glucose (MM= 180.2 g/mol), then find the molecular formula for glucose.



$$\text{\# of empirical formula units in glucose} = \frac{\text{MM of glucose}}{\text{empirical formula mass of glucose}} = \frac{180.2 \text{ g/mol}}{30.03 \text{ g/mol}} = 6.001$$

6×(CH₂O)

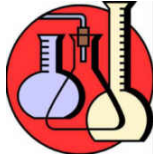
Thus, the molecular formula of glucose is C₆H₁₂O₆

Determination of the Chemical Formula from Mass Percentage

A sample was analyzed and found to contain 43.64% phosphorous and 56.36% oxygen. If the MM = 283.88 g/mol, find the empirical and molecular formula.

Chapter 3 Section 6

Stoichiometric Calculations




- **Stoichiometry** is
 - the accounting or math behind chemistry.
 - using balanced chemical equations to predict the quantity of a particular reactant or product.
- Useful web links about stoichiometry:
 - <http://dbhs.wvusd.k12.ca.us/webdocs/Stoichiometry/Stoichiometry.html>
 - <http://www.shodor.org/UNChem/basic/stoic/index.html>
 - http://www.chem.vt.edu/RVGS/ACT/notes/Study_Guide-Moles_Problems.html

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Chapter 3 Section 6

Stoichiometric Calculations



$$4\text{NH}_3(\text{g}) + 5\text{O}_2(\text{g}) \longrightarrow 4\text{NO}(\text{g}) + 6\text{H}_2\text{O}(\text{g})$$

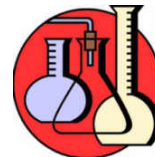
- What does this reaction mean?
 - # of atoms/molecules?
 - # of moles?
 - # of grams?

X $4\text{g NH}_3(\text{g}) + 5\text{g O}_2(\text{g}) \longrightarrow 4\text{g NO}(\text{g}) + 3\text{g H}_2\text{O}(\text{g})$

$17\text{g/mol} \times 4\text{mol}$	$32\text{g/mol} \times 5\text{mol}$	$30\text{g/mol} \times 4\text{mol}$	$18\text{g/mol} \times 6\text{mol}$
68 g	160 g	120 g	108 g
228 g		228 g	

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Stoichiometric Calculations



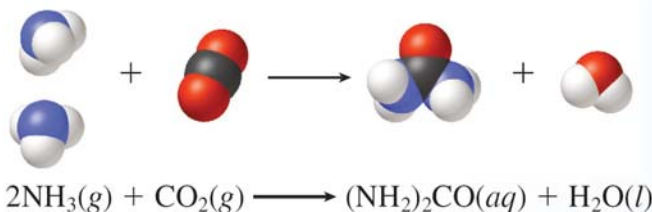
- By now, it should be clear to us that the coefficients in a chemical reaction represent **NOT** the masses of the molecules **BUT** the numbers of the molecules (or moles).
- However, in laboratory, the amounts of substances needed can not determined by counting the molecules.

Stoichiometric Calculations

Mole to Mole

Example:

How many moles of urea could be formed from 2.4 moles of ammonia?




Chapter 3 Section 6

Stoichiometric Calculations

Mass to Mass

In mass-to-mass conversion you need to:

- 1) Balance the chemical equation.
- 2) Always make the numbers of moles of the reactants and products (**the stoichiometric ratios**) to be the **reference** (the key) for your calculations.



$$1 \text{ C}_3\text{H}_8 (g) + 5 \text{ O}_2 (g) \rightarrow 3 \text{ CO}_2 (g) + 4 \text{ H}_2\text{O} (g)$$

What mass of O_2 reacts with 96.1g of C_3H_8 ?

```

    graph LR
      A[96.1 g C3H8] --> B[# mol of C3H8]
      B --> C[# mol of O2]
      C --> D[?? g of O2]
  
```

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Chapter 3 Section 6

Stoichiometric Calculations

- o What mass of O_2 reacts with 96.1g of C_3H_8 ?
- o What mass of CO_2 is produced when 96.1g of C_3H_8 is combusted with O_2 ?

$$\text{C}_3\text{H}_8 (g) + 5 \text{ O}_2 (g) \rightarrow 3 \text{ CO}_2 (g) + 4 \text{ H}_2\text{O} (g)$$

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Stoichiometric Calculations

- Exercise:
Which is more effective antacid per gram?

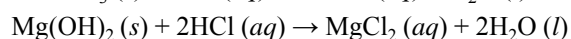
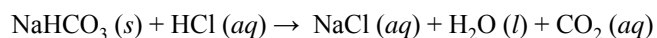


In other words, which one will react with more acid (HCl)?



Stoichiometric Calculations

Solution:



$$1.00 \text{ g NaHCO}_3 \times \frac{1 \text{ mol NaHCO}_3}{84.01 \text{ g NaHCO}_3} \times \frac{1 \text{ mol HCl}}{1 \text{ mol NaHCO}_3} = 1.19 \times 10^{-2} \text{ mol HCl}$$

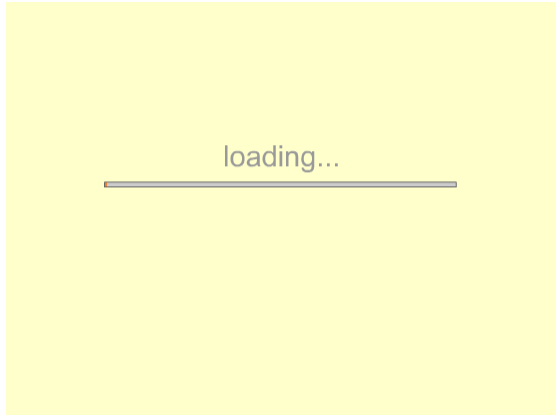
$$1.00 \text{ g Mg(OH)}_2 \times \frac{1 \text{ mol Mg(OH)}_2}{58.32 \text{ g Mg(OH)}_2} \times \frac{2 \text{ mol HCl}}{1 \text{ mol Mg(OH)}_2} = 3.42 \times 10^{-2} \text{ mol HCl}$$

Thus, Mg(OH)_2 is better antacid than NaHCO_3 per one gram.



Chapter 3 Section 7

Limiting Reactants



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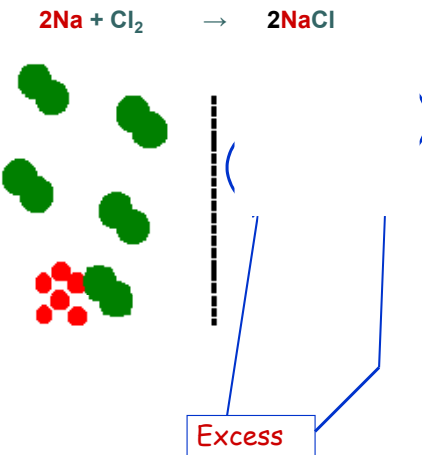
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Chapter 3 Section 7

Limiting Reactants

- Limiting reactant:**
is the reactant that is consumed fully before any other reactants. It is the reactant used for stoichiometric calculations.
- Excess:**
is the reactant that is not fully consumed in a chemical reaction.

$$2\text{Na} + \text{Cl}_2 \rightarrow 2\text{NaCl}$$



Also visit:
<http://www.science.uwaterloo.ca/~cchieh/cact/c120/limitn.html>

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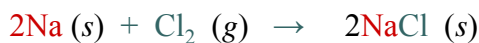
Limiting Reactants

Exercise: When 5.0 moles of hydrogen react with 5.0 moles of oxygen, how many moles of water can be produced?

Limiting Reactants

Exercise: If you put equal weights of sodium metal (Na) and chlorine gas (Cl₂) into a reaction vessel, which is going to be the limiting reagent?

Solution: Consider 1.00 g from each.



$$1.00\text{g Na} \times \frac{1 \text{ mol Na}}{22.99 \text{ g Na}} = 0.0435 \text{ mol Na}$$

$$1.00\text{g Cl}_2 \times \frac{1 \text{ mol Cl}_2}{70.90 \text{ g Cl}_2} = 0.0141 \text{ mol Cl}_2$$

1 mole of Cl₂ needs 2 moles of Na => 0.0141 mol of Cl₂ need 0.0282 mol of Na. But we have 0.0435 mol of Na (**Na is in excess** and **Cl₂ is the limiting reactant**).

Limiting Reactants

In stoichiometric calculations involving limiting reactants, follow these steps:

1. Balance the chemical equation.
2. Use the key (**# of moles of reactants and products**) to make comparison between the amount of each substance involved in the calculations.
3. Determine which reactant is the limiting one.
4. Continue with your calculations based on the limiting reactant.
5. Convert from moles into grams if you need to.



Limiting Reactants

- Ready for another exercise??

Exercise: In one process, 124 g of Al are reacted with 601 g of Fe₂O₃ According to:



Calculate the mass of Al₂O₃ formed.



Strategy:

- Make sure the equation is balanced.
- Find out which one is the limiting reactant.
- Use the limiting reactant to get the moles (then grams) for the product Al₂O₃.

Limiting Reactants



g Al we start with \rightarrow mol Al \rightarrow mol Fe_2O_3 \rightarrow g Fe_2O_3 we need.

$$124 \text{ g Al} \times \frac{1 \text{ mol Al}}{27.0 \text{ g Al}} \times \frac{1 \text{ mol Fe}_2\text{O}_3}{2 \text{ mol Al}} \times \frac{160.0 \text{ g Fe}_2\text{O}_3}{1 \text{ mol Fe}_2\text{O}_3} = 367 \text{ g Fe}_2\text{O}_3$$

124 g Al needs 367 g Fe_2O_3 , but we have 601 g Fe_2O_3 (**Fe_2O_3 is in excess**) and Al is the **limiting reactant**.

Then, g Al \rightarrow mol Al \rightarrow mol Al_2O_3 \rightarrow g Al_2O_3

$$124 \text{ g Al} \times \frac{1 \text{ mol Al}}{27.0 \text{ g Al}} \times \frac{1 \text{ mol Al}_2\text{O}_3}{2 \text{ mol Al}} \times \frac{102.0 \text{ g Al}_2\text{O}_3}{1 \text{ mol Al}_2\text{O}_3} = 234 \text{ g Al}_2\text{O}_3$$

Percent Yield

- **Theoretical Yield:** is the amount of product that would result if all the limiting reagent reacted (*very seldom!*).
- **Actual Yield:** is the amount of product actually (experimentally) obtained from the reaction.

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

Example: For the previous reaction, if one obtains 198g of Al_2O_3 , what is then the percent yield for Al_2O_3 ?

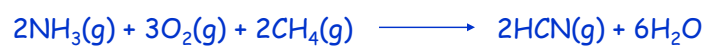
Solution:

$$\% \text{ Yield} = \frac{198 \text{ g Al}_2\text{O}_3}{234 \text{ g Al}_2\text{O}_3} \times 100\% = 84.6\%$$



Exercise

Consider the following reaction that is used to produce hydrogen cyanide (HCN):



If $5.00 \times 10^3 \text{ kg}$ each of NH_3 , O_2 and CH_4 are reacted, what mass of HCN and of H_2O will be produced, assuming 85.0% yield?