الصيغ و الحسابات الكيميائية

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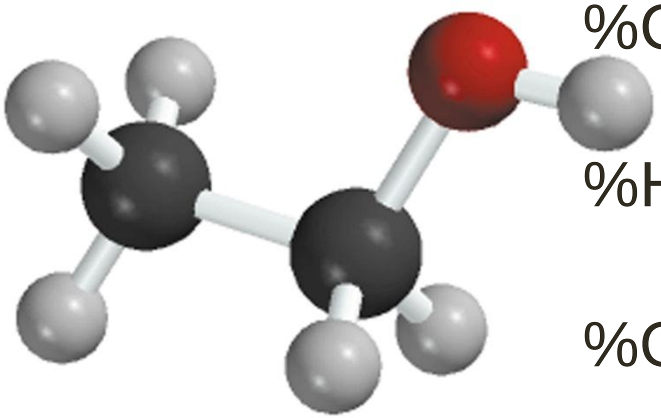
Percent composition of an element in a compound =

$$\frac{n \text{ x molar mass of element}}{\text{molar mass of compound}} \text{ x } 100\%$$

n is the number of moles of the element in 1 mole of the compound



C_2H_6O

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

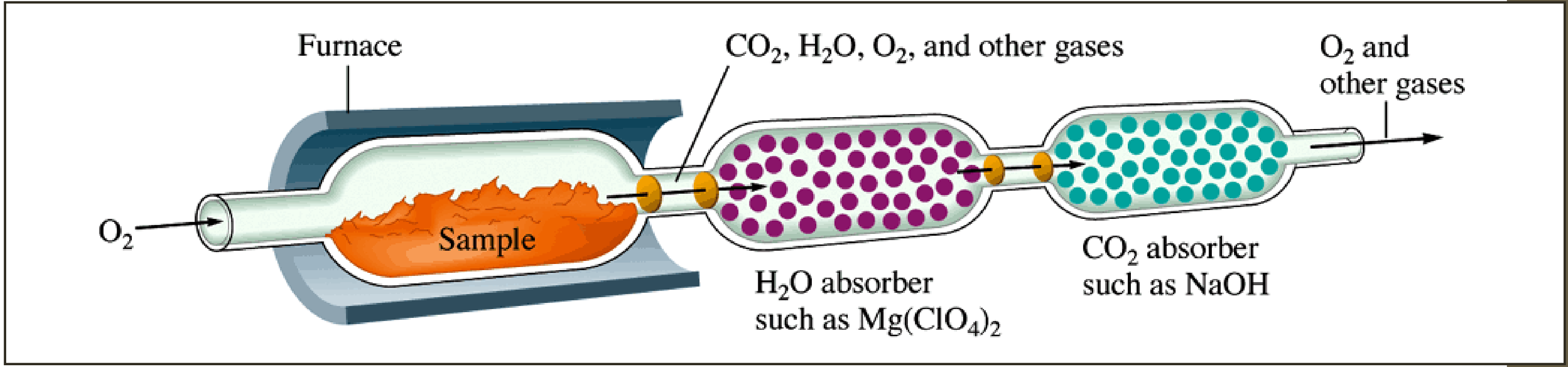
$$\%H = \frac{6 \text{ x } (1.008 \text{ g})}{46.07 \text{ g}} \text{ x } 100\% = 13.13\%$$

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

52.14% + 13.13% + 34.73% = 100.0%

Determining Elemental Composition (Formula)

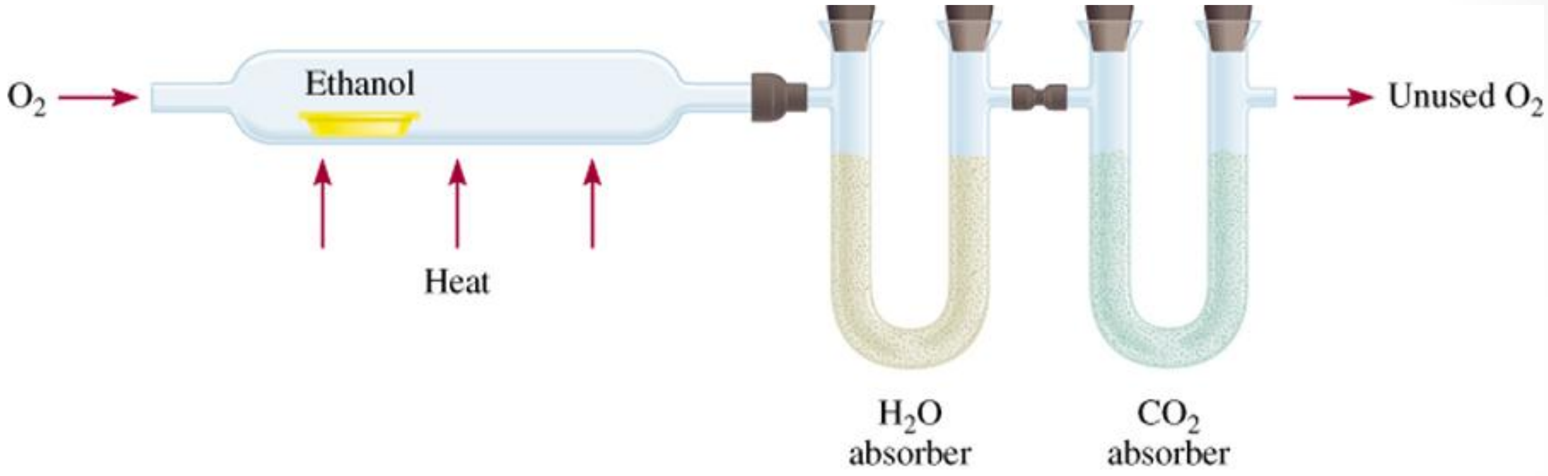
Figure 3.5: A schematic diagram of the combustion device used to analyze substances for carbon and hydrogen.



- The masses obtained (mostly CO_2 and H_2O and sometimes N_2)) will be used to determine:

1. % composition in compound
2. Empirical formula
3. Chemical or molecular formula if the Molar mass of the compound is known or given.

Example of Combustion



Combust 11.5 g ethanol

Collect 22.0 g CO_2 and 13.5 g H_2O

Collect 22.0 g CO_2 and 13.5 g H_2O

12   16 x 2

1mol CO_2 → $44gCO_2$ → 1mol C → 12g C

→ $22gCO_2$ → m_c

% C in CO_2 collected

$$m_c = \frac{22gCO_2 \times 12gC}{44gCO_2}$$

= 6g C

Convert g to mole:

$1mol\ C \longrightarrow 12g\ C$
$n_{mol}\ C \longrightarrow 6g$

$$n_c = \frac{6g \times 1molC}{12\ gC} = 0.5\ mol$$

Repeat the same for H from H_2O

$1mol\ H_2O \longrightarrow 18g\ H_2O \longrightarrow 2\ mol\ H \longrightarrow 2g\ H$

$13.5g\ H_2O \longrightarrow n_{mol}\ H \longrightarrow mH$

$$n_{mol}\ H = \frac{2x13.5}{18\ mol\ H} = 1.5\ mol\ H$$

Faster H but still need O

$$mH = \frac{2x13.5}{18} = 1.5\ g\ H$$

$$m_O = 11.5g - m_C - m_H$$
$$= 11.5 - 6 - 1.5 = 4g$$

$$n_O = \frac{m}{MM} = \frac{4}{16} = 0.25\ mol\ O$$

Empirical formula $C_{0.5}H_{1.5}O_{0.25}$

Divide by smallest subscript (0.25)

Empirical formula C_2H_6O

Then
Empirical Formula

Using the previously calculated % in compound:

a. Number of mole of C = $\dfrac{\text{\% in gram}}{\text{Atomic mass of C}}$

b. Number of mole of H = $\dfrac{\text{\% in gram}}{\text{Atomic mass of H}}$

Then divide by the smallest number: $\dfrac{a}{\text{smallest}} : \dfrac{b}{\text{smallest}} : \dfrac{c}{\text{smallest}}$

Note

- If results are : 0.99 : 2.01 : 1.00
- Then you have to convert to whole numbers:
  - 1 : 2 : 1
    - CH_2N

- If results are : 1.49 : 3.01 : 0.99
- Then you have to multiply by 2:
- 3 : 6 : 2
- $C_3H_6N_2$

Hence, empirical formula is the simplest formula of a compound

Formulas

molecular formula = (empirical formula)$_n$

[n = integer]

molecular formula = C_6H_6 = $(CH)_6$

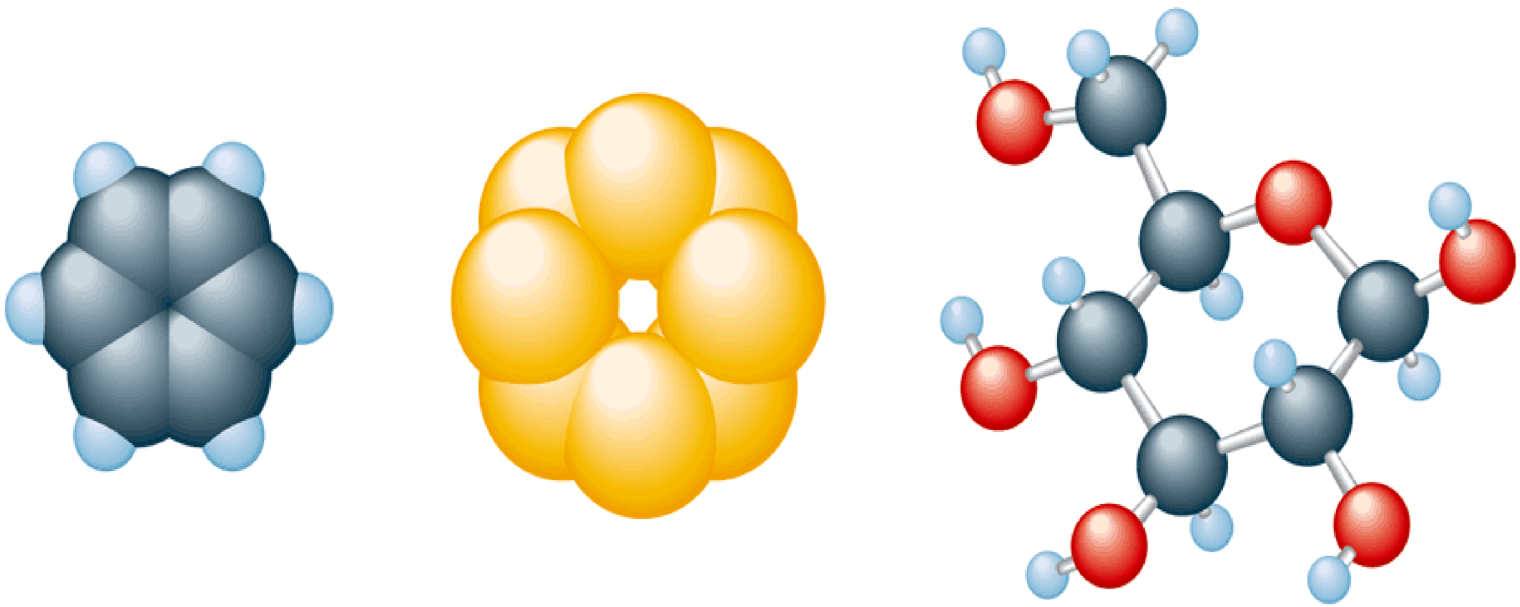
empirical formula = CH

Then

$$\frac{\text{Molecular Mass}}{\text{Empirical Mass}} = n$$

Figure 3.6:

Examples of substances whose empirical and molecular formulas differ. Notice that molecular formula = (empirical formula)n, where *n* is a integer.



$C_6H_6 = (CH)_6$ $S_8 = (S)_8$ $C_6H_{12}O_6 = (CH_2O)_6$

المتفاعل المحدد والمتفاعل الفائض والمحصول الفعلي والمحصول النظري والمحصول المئوي

إذا أدى مزج (4g) من H_2 مع (40g) من N_2 إلى الحصول على (15.45g) من NH_3، فما المتفاعل المحدد؟ وما المتفاعل الفائض؟ واحسب المحصول النظري، والمحصول المئوي.

الحل:

المعطيات: يوجد من H_2 مولان، ومن N_2 1.43 مول، وما تم الحصول عليه فعلياً هو 0.91 مول من NH_3.

المتفاعل المحدد والمتفاعل الفائض:

نكتب المعادلة، ونضع تحت كل مادة عدد المولات كما تحدده المعادلة، ذلك عدد المولات كما هو من معطيات السؤال، ثم نقسم الأخير على الأول، والمادة التي تعطي ناتج قسمة أقل تكون هي المتفاعل المحدد، والتي تعطي ناتج قسمة أكبر تكون هي المتفاعل الفائض.

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

1.00	3	عدد المولات حسب المعادلة
1.43	2	عدد المولات حسب المعطى
1.43	0.67	ناتج القسمة

ومنه يتضح أن H_2 هو المتفاعل المحدد الذي يستهلك بأكمله، وأن N_2 هو المتفاعل الفائض الذي يستهلك بعضه ويبقى جزء منه **فائضاً**.

المحصول الفعلي: هو الكمية التي نتجت فعلياً ومقدارها يتم قياسه عملياً ويعطى في المسألة وهو هنا 0.91 مول.

المحصول النظري: نكتب المعادلة، ونضع تحت المتفاعل المحدد عدد مولاته حسب المعادلة وحسب المعطى، ونضع تحت الناتج عدد مولاته حسب المعادلة:

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

3 عدد المولات حسب المعادلة **2**

2عدد المولات حسب المعطى **المحصول النظري**

المحصول النظري = $(2 \times 2)/3$

المحصول النظري = 1.33 mol

المحصول المئوي: نحسب المحصول المئوي حسب المعادلة:

المحصول المئوي = (المحصول الحقيقي / المحصول النظري) × 100

المحصول المئوي = $(0.91 / 1.33)\times100$

= المحصول المئوي 68.42 %

Limiting Reactant Calculations

What weight of molten iron is produced by 1 kg each of the reactants?

$Fe_2O_3(s)$ + $2\ Al(s) \rightarrow Al_2O_3(s) + 2\ Fe(\ell)$

$\frac{1\ \text{mol}}{6.26\text{mol}}$ $\frac{2\ \text{mol}}{18.52}$

Ratio:

0.160 **>** 0.108

Limiting Excess

The 6.26 mol Fe_2O_3 will Disappear first

Theoretical Yield is the amount of product that would result if all the limiting reagent reacted. Its amount is Calculated using the balanced equation.

Actual Yield is the amount of product actually obtained from a reaction. It is usually given.

Percent Yield

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

Actual yield = quantity of product actually obtained

Theoretical yield = quantity of product predicted by stoichiometry

Percent Yield Example

$$C_7H_6O_3(s) + C_4H_6O_3(\ell) \longrightarrow C_9H_8O_4(s) + CH_3CO_2H(\ell)$$

salicylic acid | acetic anhydride | aspirin | acetic acid

14.4 g | excess

Actual yield = 6.26 g

Sample Exercise

Titanium tetrachloride, $TiCl_4$, can be made by combining titanium-containing ore (which is often impure TiO_2) with carbon and chlorine -

$$TiO_{2(s)} + 2\ Cl_{2(g)} + C_{(s)} \rightarrow TiCl_{4(l)} + CO_{2(g)}$$

If one begins with 125 g each of Cl_2 and C, but plenty of titanium-containing ore, which is the limiting reagent in the reaction? What quantity of $TiCl_4$ can be produced?

Practice Example 3

- Nitrogen gas can be prepared by passing gaseous ammonia over solid copper(II) oxide at high temperatures. The other products of the reaction are solid copper and water vapor. If a sample containing 18.1g of NH_3 is reacted with 90.4g of CuO, which is the limiting reactant? How many grams of N_2 will be formed.

Practice Example 4

- Methanol can be manufactured by combination of gaseous carbon monoxide and hydrogen. Suppose 68.5Kg CO(g) is reacted with 8.60Kg H 2(g). Calculate the theoretical yield of methanol. If 3.57x104g CH3OH is actually produced, what is the percent yield of methanol?

Practice Example 5

- $SnO_2(s) + 2\ H_2(g) \rightarrow Sn(s) + 2\ H_2O(l)$

- a) the mass of tin produced from 0.211 moles of hydrogen gas.
- b) the number of moles of H_2O produced from 339 grams of SnO_2.
- c) the mass of SnO_2 required to produce 39.4 grams of tin.
- d) the number of atoms of tin produced in the reaction of 3.00 grams of H_2.
- e) the mass of SnO_2 required to produce 1.20×10^{21} molecules of water.