Chapter 3 - Moles, Atoms, Mass Percents and Stoichiometry

Section 2 – Mass Percent and Empirical Formula

Dr. Sapna Gupta

1

Introduction

Chemical compounds are represented as formulas. One way of knowing the formula for ionic compounds is by looking at the valancies. But as we learned in the nomenclature of covalent compounds there can be more than one compound of the two elements, e.g. NO and NO_3 or CO and CO_2. How do we determine the formulas for these compounds?

For this we need to learn about mass percents and then learn how we can use instrumentation to calculate the formulas of ionic and covalent compounds.

2

Chemical Formulas

1) Empirical Formula – Is the lowest ratio of combination of elements e.g. H_2O, CH_2O.
2) Molecular Formula – The actual ratio of elements in a compound. Generally, for ionic compounds the empirical formula is also the molecular formula (formula unit).

E.g. H_2O_2 is molecular formula and HO is the empirical formula.

In some covalent compounds the empirical formula has to be multiplied by an integer to give the molecular formula.

E.g. $(CH_2O) \times 6 = C_6H_{12}O_6$ (glucose)

3) Structural Formula – This is the 3D representation of the ionic or covalent compound.

Mass Percent

- In a compound there can be two or more elements. In mass percent calculations we calculate the mass percent of each element in that compound.
- This type of calculation is important in finding how much element might be contributing to the total mass of the compound.
- To do these calculations we first find the total mass of the compound and then find the mass of each of the elements in the compound.

$$\% \text{ mass of an element} = \frac{\text{mols of element x at. mass of element}}{\text{molar mass of the compound}} \times 100\%$$

Try to look at each compound in terms of mols. This will help you in future calculations.

For e.g. in Na_2CO_3 – there are 2 mols of sodium, 1 mol of carbon and 3 mols of oxygen.

Solved Problem: Mass percent

Silver chromate, Ag_2CrO_4, is used in lab for staining neurons. What is the percentage of each element in silver chromate?

First, find the molar mass of Ag_2CrO_4:

2 Ag	2(107.9) =	215.8
1 Cr	1(51.996) =	51.996
4 O	4(16.00) =	64.00
		331.796

Now, convert each to percent composition:

$$Ag: \quad \frac{215.8 \text{ g}}{331.796 \text{ g}} \times 100\% = \boxed{65.04\% \, Ag}$$

$$Cr: \quad \frac{51.99 \text{ g}}{331.796 \text{ g}} \times 100\% = \boxed{15.67\% \, O}$$

$$\text{O}: \quad \frac{64.00 \text{ g}}{331.796 \text{ g}} \times 100\% = \boxed{19.29\% \, O}$$

Check: all percents should add to 100%
65.04 + 15.67 + 19.29 = 100.00

5

Solved Problem: Gram of an element in gram of compound

The chemical name of table sugar is sucrose, $C_{12}H_{22}O_{11}$. How many grams of oxygen are in 68.1 g of sucrose?

First, find the molar mass of $C_{12}H_{22}O_{11}$:

12 C	12(12.01) =	144.12
11 O	11(16.00) =	176.00
22 H	22(1.008) =	22.176
		342.296 g/mol

Now, find the mass of carbon in 68.1 g sucrose:

$$68.1 \text{ g sucrose} \times \frac{176.00 \text{ g oxygen}}{342.30 \text{ g sucrose}} = \boxed{35.01 \, g \text{ oxygen}}$$

6

Solved Problem: Percent water in a hydrate

What is the percent water in copper(II) sulfate pentahydrate, $CuSO_4 \cdot 5\ H_2O$?

1 Cu	(1)63.55 g = 63.55 g			
1 S	(1)32.07 g = 32.07 g		2 H	(2)1.01 = 2.02 g
4 O	(4)16.00 g = 64.00 g		1 O	(1)16.00 =16.00 g
	159.62 g/mol			18.02 g/mol

Formula Mass of hydrate = 159.62 + 5(18.02) = 249.72 g/mol

Divide the mass of water in one mole of the hydrate by the molar mass of the hydrate and multiply this fraction by 100.

$$\text{percent hydrate} = \frac{(5 \times 18.02)}{249.72} \times 100\% = \boxed{36.08\%\ H_2O}$$

Empirical Formulas

Refer to the first couple to see the three formulas: empirical, molecular and structural.

The empirical formula of a substance written with the smallest integer subscripts.

The empirical formula for the molecular formula N_2O_4 is NO_2. (Divide both 2 and 4 by 2)

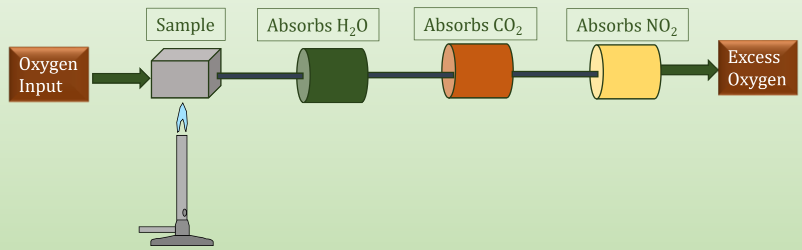
If an empirical formula is HO then the entire formula (each atom) has to be multiplied by 2 to find the molecular formula of hydrogen peroxide H_2O_2.

How do we get the empirical formula? By using elemental analysis (combustion reaction) in the lab.

How do we get the integer 2 to multiply with? This is found by mass spectrophotometer in the lab. This instruments find the mass of a substance.

Elemental Analysis

- Below shows the apparatus used for elemental analysis of a substance. Elements such as C, H, N, S and sometimes O can be anlysed.



- The sample is burned in oxygen (combustion reaction) and the products, carbon dioxide and water and other oxides are collected separately and weighed.
- The mass of the oxides are then used to calculate the weight of the element (not oxygen). This can be used to calculate the empirical formula of the compound.

9

Determining Empirical Formula

Generally, you will be given percents of each of the element in the formula.

1. Covert the percent to 100 g of the substance. (e.g. 39% C = 39 g C)
2. Convert grams to moles for each element.
3. Create the molecular formula using these moles.
4. Divide each mole amount by the smallest mole amount to get mol ratio. Now you can round off numbers.

How to Round off

- When rounding off mol ratios, 1.99 or 1.89 can be rounded to 2, but 1.49 cannot be rounded to 2 or 1.
- In case of certain decimal points the mole has to be multiplied by an integer to make whole numbers as shown below.

  For example:
  - If the decimal portion is 0.5, multiply by 2.
  - If the decimal portion is 0.33 or 0.67, multiply by 3.
  - If the decimal portion is 0.25 or 0.75, multiply by 4.

10

Determining Molecular Formula

Molecular formula is the actual ratio of elements.

- To get the molecular formula you need to know the molecular mass of the compound. This will be given to you.
- Find the molecular weight of the empirical formula.
- Divide the molecular weight by the mass of the empirical formula. Multiply the empirical formula with that number (n) obtained.

11

Solved Example: Molecular formula from empirical formula
A compound has an empirical formula of CH. The molecular mass was found to be 52.08 g/mol. What is the molecular formula of this compound?

Empirical Formula CH weight = C + H = 12.01 + 1.008 = 13.018 g/mol

$$\frac{Molecular\ weight}{Empirical\ formula\ weight} = n = \frac{52.08}{13.018} = 4$$

Molecular formula = (CH) x 4 = $\boxed{C_4H_4}$

12

Solved Problem: Calculating empirical formula

Sodium pyrophosphate is used in detergent preparations. It is composed of 34.5% Na, 23.3% P, and 42.1% O. What is its empirical formula?

Step 1: Convert all percents to grams and find mols of each element

$$34.5 \text{ g Na} \times \frac{1 \text{ mol Na}}{22.99 \text{ g Na}} = 1.501 \text{ mol Na}$$

$$23.3 \text{ g P} \times \frac{1 \text{ mol P}}{30.97 \text{ g P}} = 0.7523 \text{ mol P}$$

$$42.1 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 2.631 \text{ mol O}$$

Step 2: Divide all mols by the smallest mols found in step 1

$$\frac{1.501 \; mol\; Na}{0.7523} = 2.00 \quad \boxed{\times 2 = 4}$$

$$\frac{0.7523 \; mol\; P}{0.7523} = 1.00 \quad \boxed{\times 2 = 2}$$

$$\frac{2.631 \; mol\; O}{0.7523} = 3.50 \quad \boxed{\times 2 = 7}$$

Step 3: Multiply all mols by 2 because O is 3.5.

Empirical formula
$Na_4P_2O_7$

13

Solved Problem: Empirical and molecular formula

Benzene is composed of 92.3% carbon and 7.7% hydrogen. What is the empirical formula of benzene? Its molecular weight is 78.1 amu. What is its molecular formula?

Step 1

$$92.3 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 7.685 \text{ mol C}$$

$$7.7 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 7.64 \text{ mol H}$$

Step 2

$$\frac{7.685}{7.64} = 1$$

$$\frac{7.64}{7.64} = 1$$

Empirical formula: CH

Step 3

Empirical formula weight = 13.02 amu

$$\frac{Molecular\ weight}{emprical\ formula\ weight} = n = \frac{78.1}{13.02} = 6$$

Molecular formula: C_6H_6

Molecular formula = (CH) × n = (CH) × 6 = C_6H_6

14

Solved Problem: Empirical and molecular formula

Hexamethylene is one of the materials used to produce a type of nylon. It is composed of 62.1% C, 13.8% H, and 24.1% N. Its molecular weight is 116 amu. What is its molecular formula?

Step 1

$$62.1 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 5.171 \text{ mol C}$$

$$13.8 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 13.69 \text{ mol H}$$

$$24.1 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ g N}} = 1.720 \text{ mol H}$$

Step 2

$$\text{mol C} \quad \frac{5.171}{1.720} = 3$$

$$\text{mol H} \quad \frac{13.69}{1.720} = 8$$

$$\text{mol H} \quad \frac{1.720}{1.720} = 1$$

Empirical formula C_3H_8N

Step 3

Molecular weight of the empirical formula C_3H_8N.

3(12.01) + 8(1.008) + 1(14.01) = 58.104 amu

$$n = \frac{116}{58.10} = 2$$

Molecular formula = $(C_3H_8N \times 2)$ = $\boxed{C_6H_{16}N_2}$

Key Words and Concepts

- Mass percents
- Elemental analysis
- Empirical formula
- Molecular formula