Sections 3.3, 3.7, and 3.8

Notes from Chapter # 3 Part 3

Composition of Compounds

Representing compounds Chemical formulas and molecular formulas

Determining Chemical formula form experimental data

3.7 Composition of Compounds

Molar Mass of Compounds

 The relative masses of molecules can be calculated from atomic masses

Formula Mass = 1 molecule of H_2O

- = 2(1.01 amu H) + 16.00 amu O = 18.02 amu
- 1 mole of H_2O contains 2 moles of H and 1 mole of O so molar mass = 1 mole H_2O

$$= 2(1.01 \text{ g H}) + 16.00 \text{ g O} = 18.02 \text{ g}$$

Percent Composition

- · Percentage of each element in a compound
 - ✓ by mass

- · Can be determined from
- 1. the formula of the compound
- 2. the experimental mass analysis of the compound

 The percentages may not always total to 100% due to rounding

$$Percentage = \frac{part}{whole} \times 100\%$$

Example: Find the mass percent of Cl in C₂Cl₄F₂

Given: Find:	- 2 - 4 2		
Conceptual Plan:	Mass % CI = $\frac{4 \times \text{molar mass CI}}{\text{molar mass C}_2\text{CI}_4\text{F}_2} \times 100\%$		
Relationships:	Mass % element $X = \frac{\text{mass element } X \text{ in 1 mol}}{\text{mass 1 mol of compound}} \times 100\%$		
Solution: $4 \times \text{molar mass Cl} = 4(35.45 \text{ g/mol}) = 141.8 \text{ g/mol}$ molar mass $C_2Cl_4F_2 = 2(12.01) + 4(35.45) + 2(19.00) = 203.8 \text{ g/mol}$			
Mass % CI = $\frac{141.8 \text{ g/mol}}{203.8 \text{ g/mol}} \times 100\% = 69.58\%$			
Check:	because the percentage is less than 100 and CI is much heavier than the other atoms, the number makes sense		

Example 2 :Determine the mass percent composition of $CaCl_2$ (Ca = 40.08, Cl = 35.45)

$$\begin{array}{ll} \bullet & \text{CaCl}_2 & \text{Mass \% Ca} = \frac{\text{molar mass Ca}}{\text{molar mass CaCl}_2} \times 100\% \\ & \text{Mass \% CI} = \frac{2 \times \text{molar mass CI}}{\text{molar mass CaCl}_2} \times 100\% \\ & 2 \times \text{molar mass CI} = 2(35.45\,\text{g/mol}) = 70.90\,\text{g/mol} \\ & \text{molar mass CaCl}_2 = 1(40.08) + 2(35.45) = 110.98\,\text{g/mol} \\ & \text{Mass \% Ca} = \frac{40.08\,\text{g/mol}}{110.98\,\text{g/mol}} \times 100\% = 36.11\% \\ & \text{Mass \% CI} = \frac{70.90\,\text{g/mol}}{110.98\,\text{g/mol}} \times 100\% = 63.88\% \\ \end{array}$$

3.8 Representing compounds Chemical formulas and molecular formulas

Empirical formula	Molecular formula	Structural formula	Molecular Models (3D)
НО	$\mathrm{H_2O_2}$	Н-О-О-Н	-
CH ₃	$\mathrm{C_2H_6}$	H H H—C—C—H H H	A.
CH ₄	CH ₄	H 108.70 pm	Ball-and-stick model

Empirical Formula - A formula that gives the simplest whole-number ratio of atoms in a compound.

3.9 Steps for Determining an Empirical Formula

1. Start with the number of grams of each element, given in the problem.

o If percentages are given, assume that the total mass is 100 grams so that

the mass of each element = the percent given.

2. Convert the mass of each element to moles using the molar mass from the periodic table.

3. Divide each mole value by the smallest number of moles calculated.

4. Then multiply each solution by the same factor to get the lowest whole number multiple

This is the mole ratio of the elements and is represented by subscripts in the empirical formula.

Example Problem #1

A compound was analyzed and found to contain 13.5 g Ca, 10.8 g O, and 0.675 g H. What is the empirical formula of the compound?

Start with the number of grams of each element, given in the problem.

Given ↓

$$0.675 \, \mathrm{g} \, \mathrm{H}$$

Step 2

Convert the mass of each element to moles using the molar mass from the periodic table.

Given
$$\downarrow$$
 P.T. \downarrow

13.5 g.ea x
$$\frac{1 \operatorname{mol} Ca}{40.1 \text{ g.ea}} = 0.337 \operatorname{mol} Ca$$

10.8 g/O x
$$\frac{1 \text{ mol O}}{16.0 \text{ g/O}} = 0.675 \text{ mol O}$$

$$0.675 \text{ g.H x } \frac{1 \text{ mol Ca}}{1.01 \text{ g.H}} = 0.668 \text{ mol H}$$

Step 3

Divide each mole value by the smallest number of moles calculated.

Given
$$\downarrow$$
 P.T. \downarrow
13.5 g.Cá x $\frac{1 \mod Ca}{40.1 \text{ g.Cá}} = \frac{0.337}{0.337} \mod Ca \Rightarrow 1.00$
10.8 g.O x $\frac{1 \mod O}{16.0 \text{ g.O}} = \frac{0.675}{0.337} \mod O \Rightarrow 2.00$
0.675 g.H x $\frac{1 \mod Ca}{1.01 \text{ g.H}} = \frac{0.668}{0.337} \mod H \Rightarrow 1.98 \approx 2.00$

Is not needed her since i have only whole numbers

This is the mole ratio of the elements and is represented by subscripts in the empirical formula.

$$CaO_2H_2 \Rightarrow Ca(OH)_2$$

Example Problem #2

A compound decomposed to 57.14% C, 6.16% H, 9.52% N, and 27.18% O. Calculate the empirical formula of this compound

Step 1

If percentages are given, assume that the total mass is 100 grams so that the mass of each element = the percent given.

Given ↓

57.14 g C

6.16gH

 $9.52 \,\mathrm{g}\,\mathrm{N}$

27.18 g O

Step 2

Convert the mass of each element to moles using the molar mass from the periodic table.

Given
$$\downarrow$$
 P.T. \downarrow
57.14 g.C x $\frac{1 \text{ mol C}}{12.0 \text{ g.C}} = 4.76 \text{ mol C}$
6.16 g.H x $\frac{1 \text{ mol H}}{1.01 \text{ g.H}} = 6.10 \text{ mol H}$
9.52 g.N x $\frac{1 \text{ mol N}}{14.0 \text{ g.N}} = 0.68 \text{ mol N}$
27.18 g.O x $\frac{1 \text{ mol O}}{16.0 \text{ g.O}} = 1.70 \text{ mol O}$

Step 3

Divide each mole value by the smallest number of moles calculated.

Given
$$\downarrow$$
 P.T. \downarrow
 $57.14 \text{ g.C} \times \frac{1 \text{ mol C}}{12.0 \text{ g.C}} = \frac{4.76}{0.68} \text{ mol C} \Rightarrow 7$
 $6.16 \text{ g.H.} \times \frac{1 \text{ mol H}}{1.01 \text{ g.H.}} = \frac{6.10}{0.68} \text{ mol H} \Rightarrow 8.97 \approx 9$
 $9.52 \text{ g.N.} \times \frac{1 \text{ mol N}}{14.0 \text{ g.N.}} = \frac{0.68}{0.68} \text{ mol N} \Rightarrow 1$
 $27.18 \text{ g.O.} \times \frac{1 \text{ mol O}}{16.0 \text{ g.O.}} = \frac{1.70}{0.68} \text{ mol O} \Rightarrow 2.5$

This is the mole ratio of the elements and is represented by subscripts in the empirical formula.

Step 4

multiply each solution by the same factor to get the lowest whole number multiple.

Given
$$\downarrow$$
 P.T. \downarrow
 $57.14 \text{ g.C} \times \frac{1 \text{ mol C}}{12.0 \text{ g.C}} = \frac{4.76}{0.68} \text{ mol C} \Rightarrow 7(2) = 14$
 $6.16 \text{ g.H.} \times \frac{1 \text{ mol H}}{1.01 \text{ g.H.}} = \frac{6.10}{0.68} \text{ mol H} \Rightarrow 8.97 \approx 9(2) = 18$
 $9.52 \text{ g.N.} \times \frac{1 \text{ mol N}}{14.0 \text{ g.N.}} = \frac{0.68}{0.68} \text{ mol N} \Rightarrow 1(2) = 2$
 $27.18 \text{ g.O.} \times \frac{1 \text{ mol O}}{16.0 \text{ g.O.}} = \frac{1.70}{0.68} \text{ mol O} \Rightarrow 2.5(2) = 5$

↑ too far to round, multiply to get a whole number

Empirical formula =
$$C_{14}H_{18}N_2O_5$$

Finding molecular formula

Once the empirical formula is found, the molecular formula for a compound can be determined if the molar mass of the compound is known.

1. Simply calculate the mass of the empirical formula

2. Divide the molar mass of the compound by the mass of the empirical formula to find the ratio between the molecular formula and the empirical formula.

2. اقسم الكتله الموليه للمركب المطلوب معرفه ال molecular formula على الكتله الموليه لل empirical formula لايجاد النسبه بينهما

3. Multiply all the atoms (subscripts) by this ratio to find the molecular formula.

Example Problem #1

Calculate the molecular formula of compound has a molar mass of 294.30 g/mol and its empirical formula is $C_{14}H_{18}N_2O_5$.

The molar mass of $C_{14}H_{18}N_2O_5$

we can find the molecular formula by finding the mass of the empirical formula

$$C_{14}H_{18}N_2O_5 = 14(12.0g)+18(1.01g)+2(14.0g)+5(16.0g)=294 \text{ g/mol}$$

from P.T. \longrightarrow C H N O

Step 2

$$\frac{\text{molar mass}}{\text{empirical formula}} = \frac{294.30 \text{ g/mol}}{294 \text{ g/mol}} \approx 1$$

Step 3

$$C_{14}H_{18}N_2O_5$$
 X 1 \rightarrow $C_{14}H_{18}N_2O_5$

The molecular formula is the empirical formula

Example Problem #2

The simplest formula for vitamin C is $C_3H_4O_3$. Experimental data indicates that the molecular mass of vitamin C is about 180. What is the molecular formula of vitamin C?

First, calculate the sum of the atomic masses for $C_3H_4O_3$. Look up the atomic masses for the elements from the Periodic Table.

the sum of the atomic masses for C₃H₄O₃ is:

$$3(12.0) + 4(1.0) + 3(16.0) = 88.0 \text{ g/mol}$$

n = 180/88

n=2

molecular formula vitamin $C = 2 \times C_3H_4O_3 = C_6H_8O_6$

MORE EXAMPLES

1 # Determine the empirical formula and the molecular formula for a compound with the following elemental composition:

The molecular weight of the compound was found to be 180 g/mol.

Solution:

The first step will be to assume exactly 100 g of this substance. This means in 100 g of this compound, 40.00 g will be due to carbon, 6.72 g will be due to hydrogen, and 53.29 g will be due to oxygen.

Then convert each of these masses to moles, using their respective atomic weights

$$40.00~g~C~x~\frac{1~mol~C}{12.01~g~C}~=~3.331~mol~C$$

$$6.72 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 6.667 \text{ mol H}$$

$$53.29 \text{ g } \bigcirc \times \frac{1 \text{ mol } \bigcirc}{16.00 \text{ g } \bigcirc} = 3.331 \text{ mol } \bigcirc$$

The smallest mole quantity is either the moles of carbon or moles of oxygen (3.331 mol)

$$\frac{3.331 \text{ mol C}}{3.331 \text{ mol}} = 1.000 \text{ C} = 1 \text{ C}$$

$$\frac{6.667 \text{ mol H}}{3.331 \text{ mol}} = 2.001 \text{ H} = 2 \text{ H}$$

$$\frac{3.331 \text{ mol } \odot}{3.331 \text{ mol}} = 1.000 \odot = 1 \odot$$

Step 3

The ratio of C:H:O has been found to be 1:2:1, thus the empirical formula is: CH₂O.

Step 4

Calculate the molecular formula

$$\frac{180 \text{ g/mol}}{30 \text{ g/mol}} = 6$$

The molecular formula is a multiple of 6 times the empirical formula:

$$C_{(1\ x\ 6)}\ H_{(2\ x\ 6)}\ O_{(1\ x\ 6)}$$
 which becomes $C_6H_{12}O_6$