Session 7: LECTURE OUTLINE (SECTIONS F1-F3, pp F45 – F49 and M3, pp F91 – F93)

I. Percent Composition
   a. Definition
   b. Example

II. Empirical and Molecular Formulas
   a. Definitions
   b. Relation between the two
   c. Example

III. How to Determine Empirical Formula?
   a. Steps to use
   b. Example

IV. Combustion Analysis
   a- What is it?
   b- Its use to determine empirical formula
   c- Example

Suggested Problems: pp F45-F48 F.1A, F.2B, F.3B, F.4B, F.5A, F.5B.
p F49 F.1, F.5, F.7, F.11
p F93 M.9, M.10, M.15

PERCENT COMPOSITION

If we know the chemical formula of a compound, its composition can be expressed in terms of the percent by mass of its elements.
Remember! Percentage is the part divided by the whole times 100!

Example: Calculate the percent composition of propane, C_3H_8.

$$\% C = \frac{\text{mass of C}}{\text{mass of } C_3H_8} \times 100 = \frac{12.0\ g}{44.08\ g} \times 100 = 27.2\ \%$$

$$\% H = \frac{\text{mass of H}}{\text{mass of } C_3H_8} \times 100 = \frac{8.08\ g}{44.08\ g} \times 100 = 72.8\ \%$$

EMPIRICAL FORMULA: It is the formula that shows the smallest whole number ratio of atoms in a compound.

MOLECULAR FORMULA: It is the formula that shows the actual number of atoms present in a molecule of a molecular substance.

Molecular formula = n x empirical formula

Molecular weight = n x simplest weight

Example:
The molecular formula for benzene is C_6H_6. What is its molecular weight? Empirical formula? Empirical weight?

The molecular weight is:
6 x 12.0 amu (for the 6C's) + 6 x 1.01 amu (for the 6 H's) = 78.0 amu

The empirical formula is the simplest formula. It reflects the smallest whole number ratio by which the two elements combine.

One can easily see that the simplest formula or the empirical formula is CH.

The empirical weight is then:
12.0 amu (for C) + 1.01 amu (for H) = 13.0 amu

Note that the molecular weight is 6 times the empirical weight, just like the molecular formula is 6 times the empirical formula (n =6).

How do we determine the empirical formula?
If we know the percent composition of a compound or its elemental composition by mass, we can determine its empirical formula using the following steps:

1- Determine the mass of each element in the sample, m_x. When percentages are given, always consider 100.0 g sample.
2- Determine the number of moles of atoms of each element by using the molar mass of the element, M_x, ($n_x = m_x/M_x$).
3- Obtain the smallest whole number ratio of the atoms (the empirical formula) by dividing each number of moles of atoms by the smallest number obtained.
4- If necessary, multiply all resulting numbers by the smallest whole number to get rid of decimals.

Example1:
Hydrogen peroxide is 5.94% hydrogen and 94.06% oxygen by mass. What is its empirical formula? Knowing that its molecular weight is 34.02 amu, what is its molecular formula?

- Determine the mass of each element in the sample, m_x:
Since percentages are given we consider 100.0 g of compound, which contains 5.940 g of H and 94.06 g of O.

- Determine the number of moles of atoms of each element:
H: 5.94 g H x $\frac{1\text{mol H atoms}}{1.01\text{ g H}}$ = 5.88 mol H atoms
O: 94.06 g O x $\frac{1\text{mol O atoms}}{16.00\text{ g H}}$ = 5.78 mol O atoms

- Obtain the smallest whole number ratio of the atoms:
$\frac{5.88}{5.78}$ = 1.02 H ~ 1 H $\qquad$ $\frac{5.78}{5.78}$ = 1.00 O
The empirical formula is HO.

- Determine the molecular formula:
The empirical formula is HO and therefore, the empirical weight is (1.01 + 16.0 = 17.0 amu).
Molecular weight = n x empirical formula
$n = \frac{34.02}{17} = 2$
Molecular formula = n x empirical formula = 2(HO) = H_2O_2

COMBUSTION ANALYSIS (See Fig. M1 p F91 in your text book)

- The combustion analysis technique is used to easily determine the empirical formula of compounds containing C, H, and O.
- In this technique, excess oxygen is used to burn the sample.
- Upon combustion, all the hydrogen in the sample is converted into water and all the carbon is converted into carbon dioxide.
- If the sample contains O, part of the oxygen that is in the carbon dioxide and in water comes from the sample and the rest comes from the supplied oxygen.
- The data obtained from combustion analysis provides the mass of water and carbon dioxide obtained.
- We use this data to determine the empirical formula of the compound as follows:

1- Use the mass of water to determine the mass of H in the sample.
2- Use the mass of carbon dioxide to obtain the mass of C in the sample.
3- If the sample contains oxygen as well, we use the total mass of H and C obtained from steps 1 and 2 and subtract this from the total mass of the sample to get the mass of oxygen in the original sample (law of conservation of mass)
4- Use steps 2, 3, and 4 from the previous section on how to calculate empirical formula to determine the empirical formula of the compound.

Example: (answers and solution will be provided by TA)
Isopropyl alcohol contains C, H, and O. When we burn 11.63 g of this compound, the products are 25.5 g CO_2 and 14.0 g H_2O. The molar mass of the alcohol is 60.0 g/mol. Find its empirical and its molecular formulas.