Chemistry 201

Molecular formula
Empirical formula

NC State University

From mass ratio to stoichiometry

We can consider both calculation of the mass percent from a known chemical formula and the reverse calculation for determination of chemical formula from mass data. The most common application of these methods is for determination of unknowns or the assignment of decomposition products during thermo-gravimetric analysis. We will consider first the example of calculating the mass percent of compound. Then we will consider using mass data to determine:

1. Empirical formula
2. Molecular formula

Composition by mass

- The composition of a compound is often expressed in terms of the weight percent of each element in the compound.
- For example, ethanol has the formula C_2H_6O. One mole of ethanol has a mass of 46.07 g. The elemental formula indicates that one mole of ethanol contains two moles of carbon, six moles of hydrogen, and one mole of oxygen.

Composition by mass

- Thus the composition of the compound by mass is

$$\%\ C = \frac{2\ \text{moles C}\ (12.01\ \text{g/mole C})}{46.07\ \text{g ethanol}}\ 100\ \% = 52.14\ \%$$

Similarly the weight percents of hydrogen and oxygen in ethanol are

$$\%\ H = \frac{6\ \text{moles H}\ (1.008\ \text{g/mole H})}{46.07\ \text{g ethanol}}\ 100\ \% = 13.13\ \%$$

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

Notice that the sum of the weight percents of all the elements in a compound must equal 100 %.

Empirical vs. molecular formula

The mass percentage does not uniquely define the molecular formula. Instead it tells us the stoichiometric ratios of elements present in a molecule. For example, the empirical formula of benzene is $(CH)_n$ and mass percent data would tell us the ratio of 1:1 for carbon and hydrogen. But, these data alone would not tell us the molecular formula, namely that n = 6 for benzene. We need additional measurements from mass spectrometry or other methods to determine the molecular formula from percent mass data.

Determining molecular formula

Acetylene and benzene have the simplest formula CH. Their molar masses are 26 and 78 respectively. What are their molecular formulae?

Determining molecular formula

Acetylene and benzene have the simplest formula CH. Their molar masses are 26 and 78 respectively. What are their molecular formulae?

Solution:

1. Calculate the formula mass of the simplest formula.
CH has a mass of 13

2. Divide the molar masses by the formula mass.
Acetylene: 26/13 = 2
The chemical formula C_2H_2
Benzene: 78/13 = 6
The chemical formula C_6H_6

Determining the molecular formula

Nicotine is 74.03% C, 8.70% H, and 17.27% N.

Its M_m is 162. What is the molecular formula?

Determining the molecular formula

Nicotine is 74.03% C, 8.70% H, and 17.27% N.

Its M_m is 162. What is the molecular formula?

Solution:

1. **Multiply the molar mass by each percentage.**
   C: 0.7403 x 162 = 119.9
   H: 0.087 x 162 = 14
   N: 0.1727 x 162 = 27.9

2. **Divide each resulting fractional mass by the atomic mass of each element.**
   C: 119.9/12 = 10
   H: 14/1 = 14
   N: 27.9/14 = 2

Note that these values must be rounded to the nearest integer value.

The molecular formula is $C_{10}H_{14}N_2$