3.2 Determination of Chemical Formulas

- **Molecular formulas** – numbers of atoms of each element in a molecule
- **Empirical formulas** – relative numbers of atoms of each element using the smallest whole numbers

Example:

acetic acid → $C_2H_4O_2$ (MF) → CH_2O (EF)

formaldehyde → CH_2O (MF) → CH_2O (EF)

glucose → $C_6H_{12}O_6$ (MF) → CH_2O (EF)

Determining Empirical Formulas

- **Elemental analysis** – gives the masses of the elements in a given mass of the compound or the Mass% composition
- EF from Mass% data
  1. Consider 100 g of the compound
  2. The masses of the elements equal their mass%
  3. Convert the masses of the elements to moles
  4. Determine the relative number of moles (mol ratio)
  5. Simplify the mole ratio to whole numbers
- EF from mass data
  – Omit steps 1 and 2 above

Example:

- Determine the EF of nicotine, if the mass% of C, H and N in it are 74.0, 8.7 and 17.3 %, respectively.

1. Consider 100 g nicotine
2. **74.0 g C, 8.7 g H, 17.3 g N**
3. Convert masses to moles:

74.0 g C×(1 mol C/12.01 g C) = 6.16 mol C

8.7 g H×(1 mol H/1.008 g H) = 8.6 mol H

17.3 g N×(1 mol N/14.01 g N) = 1.23 mol N

4. Mol ratio:

6.16 mol C : 8.6 mol H : 1.23 mol N

5. Simplify the mole ratio:

(divide by the smallest number, and if necessary, multiply by a factor to get whole numbers)

$6.16/1.23 = 5.01 \cong 5$

$8.6/1.23 = 7.0 \cong 7$

$1.23/1.23 = 1.00 \cong 1$

→ simplest whole-number ratio:

5 mol C : 7 mol H : 1 mol N

→ EF:

C_5H_7N

Determining Molecular Formulas

- The MF is a whole-number multiple of the EF

$$\Rightarrow M = M_{EF} \times n$$

  - $M \rightarrow$ molar mass
  - $M_{EF} \rightarrow$ EF mass
  - $n \rightarrow$ whole number (number of EFs per molecule)

$$\Rightarrow n = M/M_{EF}$$

- Determining MFs from EFs and molar masses

Example:

- The empirical formula of nicotine is C_5H_7N and its molar mass is 162.23 g/mol. MF = ?

$$M_{EF} \rightarrow 5\times12.01+7\times1.008+1\times14.01 = 81.12 \text{ g/mol}$$

$$n = \frac{M}{M_{EF}} = \frac{162.23 \text{ g/mol}}{81.12 \text{ g/mol}} = 2.000 \cong 2$$

$$\Rightarrow MF = 2 \times EF$$

$$MF \rightarrow C_{10}H_{14}N_2$$

Combustion Analysis

- A method for elemental analysis of combustible organic compounds through their combustion in excess O_2
  - The **C** in the sample is converted to CO_2 which is absorbed in a NaOH absorber and weighed
  - The **H** in the sample is converted to H_2O which is absorbed in a P_4O_{10} absorber and weighed
  - If a third element (O, N, …), it passes through the absorbers

1 mol C from the sample → 1 mol CO_2

2 mol H from the sample → 1 mol H_2O

Example:

When 0.236 g aspirin is burned in excess O_2, 0.519 g CO_2 and 0.0945 g H_2O are formed. Determine the mass % of C, H and O in aspirin.

- **Calculate the masses of C and H in the sample based on the masses of CO_2 and H_2O:**
- **Calculate the mass of O by subtracting the masses of C and H from the total mass of the sample**

$$0.519\text{ g CO}_2 \times \left(\frac{1\text{ mol CO}_2}{44.01\text{ g CO}_2}\right) \times \left(\frac{1\text{ mol C}}{1\text{ mol CO}_2}\right) \times$$

$$\times \left(\frac{12.01\text{ g C}}{1\text{ mol C}}\right) = 0.142\text{ g C}$$

$$0.0945\text{ g H}_2\text{O} \times \left(\frac{1\text{ mol H}_2\text{O}}{18.02\text{ g H}_2\text{O}}\right) \times \left(\frac{2\text{ mol H}}{1\text{ mol H}_2\text{O}}\right) \times$$

$$\times \left(\frac{1.008\text{ g H}}{1\text{ mol H}}\right) = 0.0106\text{ g H}$$

$$0.236\text{-}0.142\text{-}0.0106\text{=}0.084\text{ g O}$$

$$\%\text{C} = \left(\frac{0.142\text{ g C}}{0.236\text{ g sample}}\right) \times 100\% = 60.0\%$$

$$\%\text{H} = \left(\frac{0.0106\text{ g H}}{0.236\text{ g sample}}\right) \times 100\% = 4.48\%$$

$$\%\text{O} = \left(\frac{0.084\text{ g O}}{0.236\text{ g sample}}\right) \times 100\% = 35.5\%$$

The empirical formula can be determined from the percentage composition in a subsequent step

3.3 Chemical Equations

- Represent chemical reactions

Reactants → Products

- Skeletal equations – show identities of reactants and products

$$H_2 + O_2 \rightarrow H_2O$$

- Law of conservation of mass
  - Atoms are neither created nor destroyed (they only change bonding partners)
  - Same atoms are present in the reactants as in the products

- Balanced chemical equations
  - same number of atoms of each element appear on each side of the equation
  - stoichiometric coefficients – needed to balance the equations

$$2H_2 + O_2 \rightarrow 2H_2O$$

  - Microscopic view

$$(2\text{ molec. }H_2 + 1\text{ molec. }O_2 \rightarrow 2\text{ molec. }H_2O)$$

  - Macroscopic view

$$(2\text{ mol }H_2 + 1\text{ mol }O_2 \rightarrow 2\text{ mol }H_2O)$$

$$(4.032\text{ g }H_2 + 32.00\text{ g }O_2 \rightarrow 36.032\text{ g }H_2O)$$

- The stoichiometric coefficients can be treated as relative number of moles of reactants and products
- Physical state symbols
  - (s) solid; (l) liquid; (g) gas; (aq) aqueous solution

$$\mathbf{2K(s) + 2H_2O(l) \rightarrow 2KOH(aq) + H_2(g)}$$

Balancing Chemical Equations

- Balancing by inspection (only simple cases)
  - Change stoichiometric coefficients only
  - Never change subscripts in formulas
  - Never add other substances to the equation

- Systematic method
  1. Write the skeletal equation
  2. Balance one element at a time using coefficients
     - Start with the elements in the most complex substance and finish with those in the least complex one
     - Alternatively, start with the element present in the fewest number of formulas and finish with the element present in the greatest number of formulas
     - Use fractional coefficients if necessary
  3. If necessary multiply the whole equation by a factor to clear the fractional coefficients
  4. Verify that the equation is balanced and the coefficients are the smallest whole numbers
  5. Specify physical states

Example: Write the balanced equation for the combustion of ethane, C_2H_6, to carbon dioxide and liquid water.

$C_2H_6 + O_2 \rightarrow CO_2 + H_2O$ **skeletal**

$C_2H_6 + O_2 \rightarrow 2CO_2 + H_2O$ **for C**

$C_2H_6 + O_2 \rightarrow 2CO_2 + 3H_2O$ **for H**

$C_2H_6 + (7/2)O_2 \rightarrow 2CO_2 + 3H_2O$ **for O**

multiply eq. by 2

$$2C_2H_6 + 7O_2 \rightarrow 4CO_2 + 6H_2O$$

$$2C_2H_6(g) + 7O_2(g) \rightarrow 4CO_2(g) + 6H_2O(l)$$

- Often polyatomic ions can be treated as single entities

Example: Balance the following skeletal eq. in aqueous solution:

$$Co(NO_3)_3 + (NH_4)_2S \rightarrow Co_2S_3 + NH_4NO_3$$

→balance Co and S:

$$2Co(NO_3)_3 + 3(NH_4)_2S \rightarrow Co_2S_3 + NH_4NO_3$$

→ balance NH_4 and NO_3:

$$2Co(NO_3)_3 + 3(NH_4)_2S \rightarrow Co_2S_3 + 6NH_4NO_3$$

→add physical state symbols:

$$2Co(NO_3)_3(aq) + 3(NH_4)_2S(aq) \rightarrow Co_2S_3(s) + 6NH_4NO_3(aq)$$