

## 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  $\rightarrow$   $C_2H_4O_2$  (MF)  $\rightarrow$   $CH_2O$  (EF)

formaldehyde  $\rightarrow$   $CH_2O$  (MF)  $\rightarrow$   $CH_2O$  (EF)

glucose  $\rightarrow$   $C_6H_{12}O_6$  (MF)  $\rightarrow$   $CH_2O$  (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:  
 $74.0 \text{ g C} \times (1 \text{ mol C} / 12.01 \text{ g C}) = 6.16 \text{ mol C}$   
 $8.7 \text{ g H} \times (1 \text{ mol H} / 1.008 \text{ g H}) = 8.6 \text{ mol H}$   
 $17.3 \text{ g N} \times (1 \text{ mol N} / 14.01 \text{ g N}) = 1.23 \text{ mol N}$

### 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)

$6.16 / 1.23 = 5.01 \cong 5$

$8.6 / 1.23 = 7.0 \cong 7$

$1.23 / 1.23 = 1.00 \cong 1$

$\rightarrow$  simplest whole-number ratio:

**5 mol C : 7 mol H : 1 mol N**

$\rightarrow$  EF:

**$C_5H_7N$**

## Determining Molecular Formulas

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

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

–  $M$  → molar mass

–  $M_{EF}$  → EF mass

–  $n$  → 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 = ?

$$M_{EF} \rightarrow 5 \times 12.01 + 7 \times 1.008 + 1 \times 14.01 = 81.12 \text{ g/mol}$$

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

$$\Rightarrow \text{MF} = 2 \times \text{EF}$$



## 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

$$0.519 \text{ g CO}_2 \times \left( \frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2} \right) \times \left( \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \right) \times \left( \frac{12.01 \text{ g C}}{1 \text{ mol C}} \right) = 0.142 \text{ g C}$$

$$0.0945 \text{ g H}_2\text{O} \times \left( \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} \right) \times \left( \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} \right) \times \left( \frac{1.008 \text{ g H}}{1 \text{ mol H}} \right) = 0.0106 \text{ g H}$$

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

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

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

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

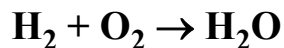
The empirical formula can be determined from the percentage composition in a subsequent step

### 3.3 Chemical Equations

- Represent chemical reactions

**Reactants → Products**

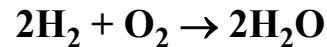
- Skeletal equations – show identities of reactants and products



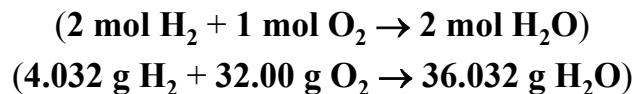
- Law of conservation of mass
  - Atoms are neither created nor destroyed (they only change bonding partners)
  - Same atoms are present in the reactants as in the products

- Balanced chemical equations

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



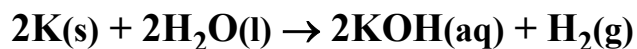
- Microscopic view  
(2 molec. H<sub>2</sub> + 1 molec. O<sub>2</sub> → 2 molec. H<sub>2</sub>O)
- Macroscopic view



– 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



### 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

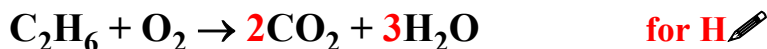
– Use fractional coefficients if necessary

3. If necessary multiply the whole equation by a factor to clear the fractional coefficients

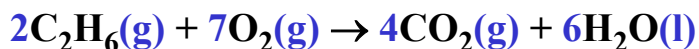
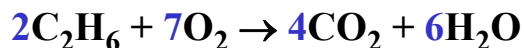
4. Verify that the equation is balanced and the coefficients are the smallest whole numbers

5. Specify physical states

**Example:** Write the balanced equation for the combustion of ethane,  $\text{C}_2\text{H}_6$ , to carbon dioxide and liquid water.

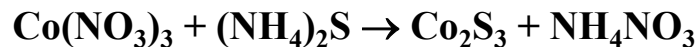


multiply eq. by 2

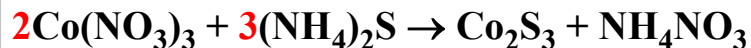


– Often polyatomic ions can be treated as single entities

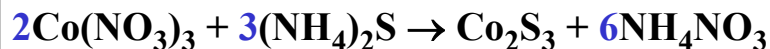
**Example:** Balance the following skeletal eq. in aqueous solution:



→balance Co and S:



→ balance  $\text{NH}_4$  and  $\text{NO}_3$ :



→add physical state symbols:

