Empirical and Molecular Formulas

Percent Composition

- The percentage by mass of any element in a compound can be found by dividing the mass of the element by the mass of the compound and multiplying by 100

$$\frac{\text{mass of element}}{\text{mass of compound}} \times 100 = \text{percent by mass}$$

- If we know the chemical formula of the compound we can calculate the percentage composition by using the molar mass
- The percentage composition will always be the same no matter how large the sample is
  - We can then assume that we have 1 mole of the substance

Example

- Determine the percent composition of Hydrogen and Oxygen in water (H_2O).
- Determine molar masses
  - $H_20 = 2(1.01) + 16 = 18.02$ g
  - $H_2 = 2(1.01) = 2.02$ g
  - O = 16 g

- Now find the percentages

$$\frac{2.02\text{ g H}}{18.02\text{ g H}_2\text{O}} \times 100 = 11.2\%\text{ H}$$

$$\frac{16\text{ g O}}{18.02\text{ g H}_2\text{O}} \times 100 = 88.8\%\text{ O}$$

Empirical Formula

- If we know the identities of the elements in a compound and the percent composition of those elements then we can determine the formula for the compound
- The empirical formula is the formula with the smallest whole number ratio of the elements
- The empirical formula may or may not be the same as the actual molecular formula

Example 1

- The percentage composition of an oxide of sulfur is 40.04% S and 59.95% O.
  - Assuming that we have 100 g of the compound we can calculate the number of moles of S and O

$$\frac{40.05\ \text{g}}{32.07\ \text{g/mol}} = 1.249\ \text{mol S}$$

$$\frac{59.95\ \text{g}}{16\ \text{g/mol}} = 3.747\ \text{mol O}$$

- Now find the lowest whole number ratio

$$\frac{1.249}{1.249} = 1\ \text{mol S}$$

$$\frac{3.747}{1.249} = 3\ \text{mol O}$$

- This gives us an empirical formula of…

SO_3

Example 2

- Experimental analysis determined that a compound contained 7.30 g of sodium (Na), 5.08 g of sulfur (S), and 7.62 g of oxygen (O).

- Find the number of moles of each

$$\frac{7.30\ \text{g}}{23\ \text{g/mol}} = 0.317\ \text{mol Na}$$

$$\frac{5.08\ \text{g}}{32\ \text{g/mol}} = 0.159\ \text{mol S}$$

$$\frac{7.62\ \text{g}}{16\ \text{g/mol}} = 0.476\ \text{mol O}$$

- Now find the lowest ratio

$$\frac{0.317}{0.159} = 2\ \text{mol Na}$$

$$\frac{0.159}{0.159} = 1\ \text{mol S}$$

$$\frac{0.476}{0.159} = 3\ \text{mol O}$$

- This gives us an empirical formula of…

Na_2SO_3

Molecular Formula

- Two (or more) different substances can have the same percentage composition and thus the same empirical formula
- However, these substances can have entirely different properties
  - In other words, they are completely different compounds
- For example, both benzene and acetylene have an empirical formula of CH

- The molecular formula specifies the actual number of atoms of each element in one molecule or formula unit of the substance
- To determine the molecular formula for a substance we must experimentally determine its molar mass
- We can then find a ratio telling us how many times larger the molecular formula is than the empirical formula

Example 1

- Benzene has an empirical formula of CH
  - Molar mass of CH = 13.02 g
- The experimentally determined molar mass of benzene is 78.12 g

$$\frac{78.12\text{ g}}{13.02\text{ g}} = 6$$

- The molecular formula should be 6 times as large as the empirical formula…

C_6H_6

Example 2

- Acetylene has an empirical formula of CH
  - Molar mass of CH = 13.02 g
- The experimentally determined molar mass of acetylene is 26.04 g

$$\frac{26.04\text{ g}}{13.02\text{ g}} = 2$$

- The molecular formula should be twice as large as the empirical formula…

C_2H_2