Empirical and Molecular Formulae

Chemistry 11

Empirical Formula:

- represents the smallest whole number ratio of atoms in a substance
- it is the simplest formula
- Ex. CH_2 , C_2H_4 , C_3H_6 , C_4H_8 , and C_5H_{10} all have one carbon atom for every two hydrogen atoms
  - $\therefore$ the empirical formula is CH2

Examples:

- What is the empirical formula of a compound consisting of 80.0% C and 20.0% H?
  1. When you are given percentages, assume a 100g sample to change the values to grams
     - $\therefore$ 80.0g C and 20.0g H
  2. Find the number of moles of each element (Don't worry about sig figs here - we will round at the end, just keep 3 or 4 digits)
  3. Divide by the lowest number of moles to find whole number ratios (sometimes this gets more complicated – see later)
  4. Write the formula

$$\text{mol C} = 80.0\text{g} \times \frac{1\text{mol}}{12.0\text{g}} = 6.67\text{mol C} \div 6.67\text{mol} = 1$$

$$\text{mol H} = 20.0\text{g} \times \frac{1\text{mol}}{1.0\text{g}} = 20.0\text{mol H} \div 6.67\text{mol} = 3$$

$\therefore$ formula $= CH_3$

- A compound contains 58.8% C, 7.3% H, and 34.1% N. What is the empirical formula of the compound?

$\therefore$ formula $= C_2H_3N$

- What is the empirical formula of a compound containing 81.8% C and 18.2% H?

$$\text{mol C} = 81.8\text{g} \times \frac{1\text{mol}}{12.0\text{g}} = 6.82\text{mol C} \div 6.82\text{mol} = 1$$

$$\text{mol H} = 18.2\text{g} \times \frac{1\text{mol}}{1.0\text{g}} = 18.2\text{mol H} \div 6.82\text{mol} = 2.67$$

- If you don't get whole numbers after dividing by the smallest mole value, multiply by a number that will give a whole number (2, 3 or 4 for our questions).
  - You can pick which number by looking at the decimal you have

$$2.67 \approx 2\frac{2}{3}$$

So multiply all numbers by the denominator (3)

$\therefore$ formula $= C_3H_8$

Molecular Formula:

- gives the actual number of atoms of each element in a molecular compound
- Found by comparing the molecular molar mass to the empirical formula mass
- Use the equations:

$$n = \frac{\text{molecular molar mass}}{\text{empirical formula mass}} \quad \text{and} \quad n(\text{empirical formula}) = \text{molacular formula}$$

Example:

- Find the molecular formula for a compound that contains 4.90g N and 11.2g O. The molar mass of the compound is 92.0g/mol?
  1. Find the empirical formula first (when not given)

$$\text{mol N} = 4.90\text{g} \times \frac{1\text{mol}}{14.0\text{g}} = 0.350\text{mol} \div 0.350\text{mol} = 1$$

$$\text{mol O} = 11.2\text{g} \times \frac{1\text{mol}}{16.0\text{g}} = 0.700\text{mol} \div 0.350\text{mol} = 2$$

$\therefore$ empirical formula = NO_2

  2. Calculate the empirical formula mass
  3. Use the molar masses to find the number of times bigger the molecular formula is compared to the empirical formula (n)
  4. Multiply the empirical formula by "n" to write the molecular formula

$$n = \frac{\text{molecular molar mass}}{\text{empirical formula mass}}$$

$$= \frac{92.0 \text{ g/mol}}{(14.0 + 16.0 + 16.0)\text{g/mol}}$$

$$= \frac{92.0 \text{ g/mol}}{46.0 \text{ g/mol}} = 2$$

Note: if you don't get a whole number here – you did something wrong!

$$n(\text{empirical formula}) = \text{molecular formula}$$

$$2(NO_2) = \text{molecular formula} = N_2O_4$$