Empirical and Molecular Formula

1. What is a molecular formula?

   The molecular formula is the actual formula of a compound. For example C_2H_6 is the actual formula for ethane.

2. What is an empirical formula?

   An empirical formula is the most reduced ratio of atoms in a compound.
   For example CH_3 would be the empirical formula for ethane.
   In the case of H_2O, the molecular formula would be the same as the empirical formula as it is already in its most reduced form.

3. How do you convert from the empirical to the molecular formula?

$$\frac{\textit{Molar Mass of the Molecular Formula}}{\textit{Molar Mass of the Empirical Formula}} = \textit{Factor}$$

   The factor tells you by what value you need to multiply the subscripts of the empirical formula to convert it into the molecular formula.

   Terephthalic acid contains C, H and O. Combustion of 19.81 mg terephthalic acid produces 41.98 mg CO_2 and 6.45 mg H_2O. If 0.250 mol of terephthalic acid has a mass of 41.5g, determine the molecular formula of terephthalic acid.

   Gather the pertinent data points.

   - 19.81 mg terephthalic acid was combusted
   - 41.98 mg of CO_2 was produced
     (this will give us information about the amount of carbon present in the original sample.)

- 6.45 mg of H_2O was produced
  (this will give us information about the amount of hydrogen present in the original sample.)

Step 1 – Determine the amount of carbon, hydrogen and oxygen present in original terephthalic acid sample.

$$41.98\ \cancel{mg}\ \frac{g}{1000\ \cancel{mg}}\ \frac{\cancel{mol\ of\ CO_2}}{44.01\ g\ \cancel{CO_2}}\ \frac{1\ \cancel{mol\ of\ C}}{1\ \cancel{mol\ CO_2}}\ \frac{12.01\ g\ C}{1\ \cancel{mol\ C}} = \boxed{0.01145\ g\ of\ Carbon}$$

$$6.45\ \cancel{mg}\ \frac{\cancel{g}}{1000\ \cancel{mg}}\ \frac{1\ \cancel{mol\ H_2O}}{18.02\ \cancel{g\ H_2O}}\ \frac{2\ \cancel{mol\ H}}{1\ \cancel{mol\ H_2O}}\ \frac{1.01\ g\ H}{1\ \cancel{mol\ H}} = \boxed{7.230 \times 10^{-4}\ g\ Hydrogen}$$

As there were no sources, other than the terephthalic acid, for the C and H. The amounts of the C and H contained in the CO_2 and H_2O are the same as the amounts contained in the original sample.

How about the oxygen?

Since the compound is only made up of C,H and O. The sum of the individual masses of each must equal the total mass sample so….

0.01981 g terephthalic acid – 0.01145 g C – 7.230×10^{-4} g H = 0.007637 g O

Step 2 – As the formula is a mole ratio of the various elements convert from mass to moles.

$$0.01145\ g\ C \times \frac{1\ mole\ C}{12.01\ g\ C} = \boxed{9.534 \times 10^{-4}\ moles\ C}$$

$$7.230 \times 10^{-4}\ g\ H \times \frac{1\ mol\ H}{1.01\ g\ H} = \boxed{7.158 \times 10^{-4}\ moles\ H}$$

$$0.007637\ g\ O \times \frac{1\ mol\ O}{16.00\ g\ O} = \boxed{4.773 \times 10^{-4}\ moles\ O}$$

Step 3 – Solve for the smallest whole number ratio between the values of moles determined in the previous step.

$$\frac{9.534 \times 10^{-4}}{4.773 \times 10^{-4}} = 2$$

$$\frac{7.158 \times 10^{-4}}{4.773 \times 10^{-4}} = 1.5$$

$$\frac{4.773 \times 10^{-4}}{4.773 \times 10^{-4}} = 1$$

$$\left.\begin{matrix}2\\1.5\\1\end{matrix}\right\} \times 2 = \left\{\begin{matrix}4\ mol\ C\\3\ mol\ H\\2\ mol\ O\end{matrix}\right.$$

Empirical Formula

$\boxed{C_4H_3O_2}$

Step 4 – Solve for the factor using the formula below. Multiply the mole ratio of the empirical formula by the factor to determine the molecular formula.

$$\frac{Molar\ Mass\ of\ the\ Molecular\ Formula}{Molar\ Mass\ of\ the\ Empirical\ Formula} = Factor$$

The problem indicated that .250 moles of terephthalic acid had a mass of 41.5g. This information indicates the molar mass. Remember that MM=g/mol so….

$$\frac{41.5g}{0.250\ mol} = 166\ g/mol$$

$$\frac{166\ g/mol}{83.07\ g/mol} = 2$$

Molecular Formula

$$\boxed{C_8H_6O_4}$$