Empirical and Molecular Formula Calculations

Empirical Formula: tells you the simplest ratio of the atoms that form a compound (must be in lowest terms) eg NaCl, $MgCl_2$, Fe, CH_2O, H_2O

Molecular Formula: tells you the exact number of each type of atom in a compound (is applicable to discrete covalent molecules only) eg $C_6H_{12}O_6$, $H_2C_2O_4$, H_2O, CH_2O

Note that a molecular formula for small molecules can be the same as the empirical formula as long as the molecular formula tells you the exact number of atoms in a molecule.

Empirical Formula Calculation:

eg 1 determine the empirical formula for a compound that is 39.99 % C, 6.73 % H and 53.28 % O by mass.

In a 100 g sample: (makes the calculation easier)

$$C: 39.99\text{ g} \times \frac{1\text{ mol}}{12.01\text{ g}} = 3.330\text{ mol} \div 3.330\text{ mol}^{*} = 1.000 \simeq 1^{**}$$

$$H: 6.73\text{ g} \times \frac{1\text{ mol}}{1.01\text{ g}} = 6.663\text{ mol} \div 3.330\text{ mol} = 2.001 \simeq 2$$

$$O: 53.28\text{ g} \times \frac{1\text{ mol}}{16.00\text{ g}} = 3.330\text{ mol} \div 3.330\text{ mol} = 1.000 \simeq 1$$

Therefore the empirical formula is CH_2O

* always divide by the smallest amount (in mol)

** round as appropriate

eg 2 determine the empirical formula for a compound that is 19.93 % C, 1.68 % H and 78.43 % Cl by mass.

In a 100 g sample:

$$C: \; 19.93\ \text{g} \times \frac{1\ \text{mol}}{12.01\ \text{g}} = 1.659\ \text{mol} \div 1.659\ \text{mol} = 1.000 \times 3^{*} = 3.000 \simeq 3$$

$$H: \; 1.68\ \text{g} \times \frac{1\ \text{mol}}{1.01\ \text{g}} = 1.663\ \text{mol} \div 1.659\ \text{mol} = 1.002 \times 3 = 3.006 \simeq 3$$

$$Cl: \; 78.43\ \text{g} \times \frac{1\ \text{mol}}{35.45\ \text{g}} = 2.212\ \text{mol} \div 1.659\ \text{mol} = 1.333 \times 3 = 4.000 \simeq 4$$

Therefore the empirical formula is $C_3H_3Cl_4$

* an extra multiplication step is required to create whole number ratios (rounding to whole numbers in the last step must always be close)

Molecular Formula Calculation:

require extra information that gives the molecular or molar mass of the compound in question.

eg 3 determine the molecular formula for a compound that is 54.52 % C, 9.17 % H and 36.31 % O by mass and has a molecular mass of 132.18 g/mol

In a 100 g sample:

$$C: 54.52\ g \times \frac{1\ mol}{12.01\ g} = 4.540\ mol \div 2.269\ mol = 2.001 \simeq 2$$

$$H: 9.17\ g \times \frac{1\ mol}{1.01\ g} = 9.079\ mol \div 2.269\ mol = 4.001 \simeq 4$$

$$O: 36.31\ g \times \frac{1\ mol}{16.00\ g} = 2.269\ mol \div 2.269\ mol = 1.000 \simeq 1$$

Therefore the empirical formula is C_2H_4O

The empirical mass is:

C: 2 x 12.01 g = 24.02 g
H: 4 x 1.01 g = 4.04 g
O: 1 x 16.00 g = 16.00 g
44.06 g

Number of Empirical Units are:

$$\frac{\text{molecular mass}}{\text{empirical mass}} = \frac{132.18\ g}{44.06\ g} = 3$$

Therefore the molecular formula is: $3 \times (C_2H_4O) = C_6H_{12}O_3$