

**WEEK 1**

## Section 1.4

## Empirical formula and molecular formula

An **empirical formula** shows the simplest ratio of elements in a compound.

A **molecular formula** shows the number of atoms of each element in a compound.

For example, for ethanoic acid (also called acetic acid), the empirical formula is  $\text{CH}_2\text{O}$  and the molecular formula is  $\text{C}_2\text{H}_4\text{O}_2$  ( $\text{CH}_3\text{CO}_2\text{H}$ ).

The empirical formula can be determined by combustion (elemental) analysis.

## Combustion analysis

As the name suggests, a known amount of a sample is heated in a furnace (to around  $1000^\circ\text{C}$ ) in the presence of oxygen and all of the carbon in the sample is converted to carbon dioxide, hydrogen is converted to water, nitrogen to nitrogen gas and/or oxides of nitrogen and sulfur to sulfur dioxide. The mixture of gaseous products is then carried by an inert carrier gas such as helium and passed over hot (around  $600^\circ\text{C}$ ) high purity copper. The copper removes any oxygen gas that has not reacted as well as converting and nitrogen oxides to nitrogen gas. The gases ( $\text{CO}_2$ ,  $\text{N}_2$ ,  $\text{SO}_2$ ,  $\text{H}_2\text{O}$ ) are then detected and quantified (the instrument is calibrated with the analysis of standard samples containing known amounts of C, H, N and/or S). Knowing the mass of the initial sample and the masses of  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{N}_2$  and/or  $\text{SO}_2$  formed on combustion allows the percentage composition of the sample to be determined (i.e. the % C, H, N and/or S). The percentage of oxygen can be determined by subtracting the mass of C, H, N and/or S from the mass of the original sample.

## Calculating the empirical formula

The elemental analysis gives the % of the various elements in the compound, which we can use to find their relative number of moles and hence the compound's empirical formula.

Here is an example to explain the calculation.

**An unknown compound contains 40.92% carbon, 4.58% hydrogen and 54.50% oxygen. Determine the empirical formula.**

(The relative atomic mass of C =  $12.01\text{ g mol}^{-1}$ , H =  $1.01\text{ g mol}^{-1}$ , O =  $16.00\text{ g mol}^{-1}$ )

Suppose the mass of the unknown compound is 100 g.  
The % C in the unknown compound is 40.92% = 40.92 g  
The % H in the unknown compound is 4.58% = 4.58 g  
The % O in the unknown compound is 54.50% = 54.50 g

As the molar mass of C is  $12.01 \text{ g mol}^{-1}$ , the number of moles of carbon in the unknown sample =  $40.92 \text{ (g)} / 12.01 \text{ (g mol}^{-1}) = 3.41 \text{ mol}$

As the molar mass of H is  $1.01 \text{ g mol}^{-1}$ , the number of moles of hydrogen in the unknown sample =  $4.58 \text{ (g)} / 1.01 \text{ (g mol}^{-1}) = 4.54 \text{ mol}$

As the molar mass of O is  $16.00 \text{ g mol}^{-1}$ , the number of moles of oxygen in the unknown sample =  $54.50 \text{ (g)} / 16.00 \text{ (g mol}^{-1}) = 3.41 \text{ mol}$

We then determine the simplest whole number ratio by dividing by the smallest molar amount (i.e. 3.41).

For C,  $3.41 / 3.41 = 1.00$

For H,  $4.54 / 3.41 = 1.33$

For O,  $3.42 / 3.41 = 1.00$

As we cannot have a fractional amount of an atom in a compound, we need to multiple the 1.33 to give an integer. Multiplying by 3 gives,

C ( $1 \times 3$ ) : H ( $1.33 \times 3$ ) : O ( $1 \times 3$ )  $\approx 3 : 4 : 3$

So, the empirical formula of the unknown compound is  $\text{C}_3\text{H}_4\text{O}_3$ .

## Determining the molecular formula

To do this we need both the empirical formula and the molecular mass ( $M_r$ ) of the unknown sample. The molecular mass of the sample can be determined by various measurement techniques, including an analytical technique called mass spectrometry.

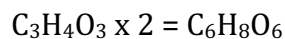
We will use both the empirical formula ( $\text{C}_3\text{H}_4\text{O}_3$ ) from above, and the fact that the unknown sample has a molecular mass of  $176.12 \text{ g mol}^{-1}$ , to explain the calculation.

The molecular mass of the empirical formula,  $\text{C}_3\text{H}_4\text{O}_3 =$   
 $(3 \times 12.01) + (4 \times 1.01) + (3 \times 16.00) = 88.07 \text{ g mol}^{-1}$

We now calculate the ratio of the molecular mass of the unknown sample to the molecular mass of the empirical formula =

$$176.12 \text{ (g mol}^{-1}\text{)} / (88.07 \text{ g mol}^{-1}\text{)} = 2$$

So, the empirical formula is one half of the actual molecular mass, and so we multiply the empirical formula by 2 to give the molecular formula;



The molecular formula is  $\text{C}_6\text{H}_8\text{O}_6$ .

## Practice makes perfect

Now have a go at this problem.

**NutraSweet contains 57.14% C, 6.16% H, 9.52% N, and 27.18% O and has the molecular mass  $294.30 \text{ g mol}^{-1}$ . Calculate the empirical formula and use this to determine the molecular formula.**

(The relative atomic mass of C =  $12.01 \text{ g mol}^{-1}$ , H =  $1.01 \text{ g mol}^{-1}$ , N =  $14.00 \text{ g mol}^{-1}$ , O =  $16.00 \text{ g mol}^{-1}$ )

### Answer

The number of moles of carbon in the unknown sample =  $57.14 \text{ (g)} / 12.01 \text{ (g mol}^{-1}\text{)}$   
= 4.76 mol

The number of moles of hydrogen in the unknown sample =  $6.16 \text{ (g)} / 1.01 \text{ (g mol}^{-1}\text{)}$   
= 6.10 mol

The number of moles of nitrogen in the unknown sample =  $9.52 \text{ (g)} / 14.00 \text{ (g mol}^{-1}\text{)}$   
= 0.68 mol

The number of moles of oxygen in the unknown sample =  $27.18 \text{ (g)} / 16.00 \text{ (g mol}^{-1}\text{)}$   
= 1.70 mol

For C,  $4.76 / 0.68 = 7.00$

For H,  $6.10 / 0.68 = 8.97 \sim 9.00$

For N,  $0.68 / 0.68 = 1.00$

For O,  $1.70 / 0.68 = 2.50$

Multiplying by 2 gives,

C (7 x 2) : H (9 x 2) : N (1 x 2) : O (2.5 x 2)  $\approx 14 : 18 : 2 : 5$

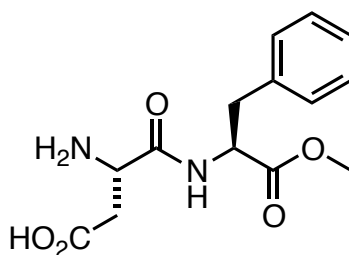
The **empirical formula** of the unknown compound is **C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>**.

The molecular mass of the empirical formula, C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub> =  
 $(14 \times 12.01) + (18 \times 1.01) + (2 \times 14.00) + (5 \times 16.00) = 294.32 \text{ g mol}^{-1}$

The given molecular mass is  $294.30 \text{ g mol}^{-1}$ , so the **molecular formula** is also **C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>**.

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Here is the structure for NutraSweet, a trade name for a compound called aspartame.



It is worth checking to make sure the structure matches the molecular formula. This artificial sweetener is 200 times sweeter than common sugar (or sucrose).