

$$\text{mol} = \frac{\text{mass}}{\text{Formula mass}}$$

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Deriving the molecular formula.

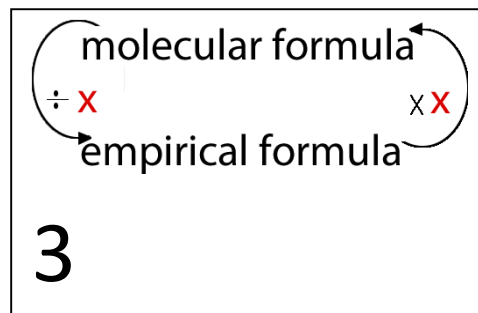
The molecular formula represents the exact number of atoms of each element in the compound whereas the empirical formula is the simplest ratio of the number of atoms of each element present.

eg. Glucose has a molecular formula of $\text{C}_6\text{H}_{12}\text{O}_6$. That is, in every molecule of glucose we have 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms. Its empirical formula, however, is CH_2O .

To find the molecular formula of a compound we first of all need to find the empirical formula and some or all the formulae above.

$$\frac{\text{formula mass}}{\text{empirical mass}} = X$$

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Let's do two examples

- Given the empirical formula of a compound is BH_3 find the molecular formula if its formula mass is 27.6 amu.

Step 1 – Since the empirical formula is given then we find “x” using the formula above.
 $\Rightarrow \text{empirical mass} = (\text{B} + 3 \times \text{H}) = (10.8 + 3) = 13.8$
 $\Rightarrow x = 27.6 / 13.8 = 2$

Step 2 Find the molecular formula
 $\Rightarrow \text{BH}_3 \times 2 = \text{B}_2\text{H}_6$
- Glucose was analysed and found to contain the following percentage composition, by mass, carbon 40.0 % oxygen 53.3 % hydrogen 6.7 %. Find the molecular formula of glucose if 3.60 grams of the pure substance contains an amount of 0.0200 mol of glucose.

Step 1 Find the empirical formula of glucose.
 find the mass of each element
 $\Rightarrow 40.0 \text{ g of C} : 53.3 \text{ g of O} : 6.7 \text{ g of H}$
 Find the mol of each element
 $\Rightarrow 40.0 / 12 \text{ C} : 53.3 / 16 : 6.7 / 1 / \text{H}$
 $\Rightarrow 3.33 \text{ C} : 3.33 \text{ O} : 6.7 \text{ H}$
 Find the simplest ratio
 $\Rightarrow 1 \text{ C} : 1 \text{ O} : 2 \text{ H} \Rightarrow \text{CH}_2\text{O}$

Step 2 Find the multiplication factor (“x”) needed to multiply the empirical formula by to derive the molecular formula
 “x” = formula mass / empirical mass
 Since we are not given the formula mass we need to calculate it using formula (1) above.
 $\Rightarrow F_m = \text{mass} / \text{mol} = 3.60 / 0.0200 = 180 \text{ amu} \Rightarrow \text{now we can find “x” } (180 / 30) = 6$
 $\Rightarrow \text{molecular formula is } (\text{CH}_2\text{O}) \times 6 = \text{C}_6\text{H}_{12}\text{O}_6$

- 1) An unknown compound composed of hydrogen, carbon and oxygen whose molecular weight has been determined to be 120 provided the following analytical results of its percentage composition, by mass.
40.0 % carbon : 6.7 % hydrogen : 46.7% oxygen.
Determine the molecular formula for this compound.

Step 1 Find the empirical formula of this compound.

$$\Rightarrow 40.0/12 \text{ C} : 6.7/1 \text{ H} : 46.7/16 \text{ O}$$

$$\Rightarrow 3.33\text{C} : 6.7 \text{ H} : 3.33 \text{ O}$$

$$\Rightarrow \text{CH}_2\text{O}$$

Step 2 Find X where

$$\Rightarrow x = \text{molecular mass} / \text{empirical mass}$$

$$\Rightarrow x = 120 / 30 = 4$$

Step 3 Find the molecular formula

$$\Rightarrow (\text{CH}_2\text{O}) \times 4 = \text{C}_4\text{H}_8\text{O}_4$$

- 2) A 100 g sample of an unknown compound was analysed and found to contain, 38.7 g of carbon, 9.8 g of hydrogen and 51.5 g of oxygen. If an amount of 0.200 mol of this substance has a mass of 12.4 grams find the molecular formula of the unknown compound.

Step 1 Find the empirical formula of this compound.

$$\Rightarrow 38.7/12 \text{ C} : 9.8/1 \text{ H} : 51.5/16 \text{ O}$$

$$\Rightarrow 3.22\text{C} : 9.8\text{H} : 3.22 \text{ O}$$

$$\Rightarrow \text{CH}_3\text{O}$$

Step 2 Find the molecular mass (formula mass)

$$F_m = \text{mass} / \text{mol}$$

$$\Rightarrow 12.4 / 0.200 = 62 \text{ g/mol}$$

Step 3 Find X where

$$\Rightarrow x = \text{molecular mass} / \text{empirical mass}$$

$$\Rightarrow x = 62 / 31 = 2$$

Step 3 Find the molecular formula

$$\Rightarrow (\text{CH}_3\text{O}) \times 2 = \text{C}_2\text{H}_6\text{O}_2$$

- 3) Nicotine, which is responsible for the addiction caused by cigarettes, has the percentage composition, by mass, 74.02% C, 8.710% H, and 17.27% N. If an amount of 0.500 mol of nicotine has a mass of 81.14 g find its molecular formula.

Step 1 Find the empirical formula of this compound.

$$\Rightarrow 74.2/12 \text{ C} : 8.7/1 \text{ H} : 17.27/14 \text{ N}$$

$$\Rightarrow 6.18\text{C} : 8.7\text{H} : 1.23 \text{ N}$$

$$\Rightarrow \text{C}_5\text{H}_7\text{N}$$

Step 2 Find the molecular mass (formula mass)

$$F_m = \text{mass} / \text{mol}$$

$$\Rightarrow 81.14 / 0.500 = 162.3 \text{ g/mol}$$

Step 3 Find X where

$$\Rightarrow x = \text{molecular mass} / \text{empirical mass}$$

$$\Rightarrow x = 162.3 / 81 = 2$$

Step 3 Find the molecular formula

$$\Rightarrow (\text{C}_5\text{H}_7\text{N}) \times 2 = \text{C}_{10}\text{H}_{14}\text{N}_2$$

- 4) Vitamin C, when analysed, is found to contain the following percentage composition by mass. 40.92% C: 54.50% O : 4.58% H. Find its molecular formula if 6.02×10^{21} molecules of Vitamin C have a combined mass of 1.76 grams.

Step 1 Find the empirical formula of this compound.

$$\Rightarrow 40.92/12 \text{ C} : 4.58/1 \text{ H} : 54.50/16 \text{ O}$$

$$\Rightarrow 3.41 \text{ C} : 4.58 \text{ H} : 3.40 \text{ O}$$

$$\Rightarrow \text{CH}_{1.33}\text{O}$$

$$\Rightarrow (\text{CH}_{1.33}\text{O}) \times 3 = \text{C}_3\text{H}_4\text{O}_3$$

Step 2 Find the molecular mass (formula mass)

$$F_m = \text{mass} / \text{mol}$$

$$\Rightarrow 6.02 \times 10^{21} = 0.010 \text{ mol}$$

$$\Rightarrow 1.76 / 0.0100 = 176 \text{ g/mol}$$

Step 3 Find X where

$$\Rightarrow x = \text{molecular mass} / \text{empirical mass}$$

$$\Rightarrow x = 176 / 88 = 2$$

Step 3 Find the molecular formula

$$\Rightarrow (\text{C}_3\text{H}_4\text{O}_3) \times 2 = \text{C}_6\text{H}_8\text{O}_6$$