

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 $C_6H_{12}O_6$. 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.

formula mass = X empirical mass 2 molecular formula * x x x empirical formula 3

Let's do two examples

- Given the empirical formula of a compound is BH₃ 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.
 => empirical mass = (B + 3 x H) = (10.8 + 3) = 13.8
 => x = 27.6 / 13.8 = 2
 Step 2 Find the molecular formula
 => BH₃ X 2 = B₂H₆
- 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

=> 40.0 g of C : 53.3 g of O : 6.7 g of H Find the mol of each element

=> 40.0 / 12 C : 53.3 / 16 : 6.7 /1/ H

=> 3.33 C : 3.33 O : 6.7 H

Find the simplest ratio

=>1C:1O:2H =>CH₂O

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. => $F_m = mass / mol = 3.60 / 0.0200 = 180 amu => now we can find "x" (180 / 30) = 6$ => molecular formula is (CH₂O) X 6 = C₆H₁₂O₆ 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.

2) 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.

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.

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 X 10²¹ molecules of Vitamin C have a combined mass of 1.76 grams.