Empirical formulae.

An empirical formula is the simplest mol ratio of elements present in a compound. As long as we know the percentage composition of the compound or the mass of each element present in a given mass of the compound then we can find the empirical formula. Below are two examples.

Example 1 - An organic compound was analysed and found to contain the following percentage composition by mass. 59.9% C, 8.1% H, 32.0% O. Calculate its empirical formula.
Follow the steps below
Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.
59.9 g of C : 8.1 g of H : 32.0 g of O
Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.
59.9/12.0 C : 8.1/1.0 H : 32.0/16 O
=> 5.0 C : 8.1 H : 2.0 O
Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.
Divide all by the lowest number of mol (2.0)
5.0/2.0 C : 8.1/2.0 H : 2.0/2.0 O
2.5C:4H:O
Step 4 Multiply to remove any fractions
It is clear from the ratio that the numbers are nowhere near whole numbers and hence we cannot simply round up or down. Here we have 2.5 mol of carbon for every 4 mol of hydrogen and 1mol of oxygen. We therefore remove the fraction by multiplying the entire ratio by 2.

$C_5H_8O_2$

Example 2- A 5.82 grams sample of an unknown oxide of aluminium (Al_xO_y) was analysed and found to contain 3.08 grams of aluminium. Calculate its empirical formula.
Follow the steps below
Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.
Since we are given masses and not percentages we must do some simple calculations first to find the mass of each element. We know that given 5.82 grams of the substance, 3.08 grams of aluminium is present. We can now find the mass of oxygen 2.74 (5.82 – 3.08) grams, since oxygen is the only other element present.
Step 2 Calculate the mol of each element present by dividing the mass of each element by its relative atomic mass.
3.08/27.0 Al : 2.74/16.0 O
=> 0.114 Al : 0.171 O
Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.
0.114/0.114 Al : 0.171/0.114 O
1 Al : 1.5 O
Step 4 Multiply to remove any fractions
It is clear from the ratio that the numbers are nowhere near whole numbers and hence we cannot simply round up or down. Here we have 1.5 mol of oxygen for every mol of aluminium. We therefore

remove the fraction by multiplying the entire ratio by 2.

$Al_1O_{1.5} = Al_2O_3$

Empirical formulae exercises

1) A polymer is a large molecule composed of smaller repeating units and so has a relatively simple empirical formula. Below are some polymers, usually plastics with their percentage composition. Calculate the empirical formula of each.

(a) Poly(methyl methacrylate), also known as acrylic or acrylic glass: 59.9% C, 8.06% H, 32.0% O
This was done as example 1 .Refer to example 1 above.
(b) *Polyvinylidene chloride was the predecessor to polyethylene or Cling Wrap*; 24.8% C, 2.0% H, 73.2% Cl
Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.
24.8 of C : 2.0 g of H : 73.2 g of Cl
Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.
24.8/12 C : 2.0/1.0 H : 73.2/35.5 of Cl
=> 2.1C : 2.0 H : 2.1Cl
Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.
Divide all by the lowest number of mol (2.0)
2.1/2.0 C : 2.1/2.0 H : 2.1/2.0 Cl
=> 1.05C : 1.0 H : 1.05 Cl
Step 4 Multiply to remove any fractions
Since there are no fractions and the mol of each element was close to a whole number, this step is not required.

$CHCl$

(c) polyethylene; 86% C, 14% H

Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.
86g of C : 14 g of H
Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.
86/12 C : 14/1.0 H
=> 7.2C : 14 H
Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.
Divide all by the lowest number of mol (7.2)
7.2/7.2 C : 14/7.2 H
=> 1C : 1.94 H
Step 4 Multiply to remove any fractions
Since there are no fractions and the mol of each element was close to a whole number, this step is not required.

CH_2

(d) polystyrene; 92.3% C, 7.7% H

Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.

92.3g of C : 7.7 g of H

Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.

92.3/12 C : 7.7/1.0 H

=> 7.7C : 7.7 H

Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.

Divide all by the lowest number of mol (7.7)

7.7/7.7 C : 7.7/7.7H

=> 1C : 1 H

Step 4 Multiply to remove any fractions

Since there are no fractions and the mol of each element was close to a whole number, this step is not required.

CH

(e) Orlon is a strong polymer used to make knitting threads; 67.9% C, 5.70% H, 26.4% N

Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.

67.9g of C : 5.70 g of H : 26 g of N

Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.

67.9g/12.0 C : 5.70/1.0 H : 26/14.0 of N

=> 5.7 C: 5.7 H : 1.9 N

Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.

Divide all by the lowest number of mol (1.9)

5.7 / 1.9 C: 5.7/1.9 H : 1.9/1.9 N

=> 3C : 3H: 1N

Step 4 Multiply to remove any fractions

Since there are no fractions and the mol of each element was a whole number, this step is not required.

C_3H_3N

2) A gaseous hydrocarbon is used in the welding of metal. Determine its empirical formula if it contains 92.3% carbon, by mass.

Solution

3) P.V.C. is used to make plastic drain pipes. When analysed it is found to contain 4.84% hydrogen, 38.4%carbon and 56.7% chlorine, by mass. What is its empirical formula?

Solution

4) A 5.23 gram sample of iron oxide was analysed and was found to contain 3.68 grams of iron. Calculate the empirical formula of this oxide.
Solution

5) When 3.90 grams of iron is burned in oxygen 5.00 grams of an oxide of iron is formed. What is the empirical formula of the oxide?
Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.
Since we are given masses and not percentages we must do some simple calculations first to find the mass of each element. We know that given 5.00grams of the iron oxide, 3.90 grams of iron is present. We can now find the mass of oxygen 1.1 (5.00 – 3.90) grams, since oxygen is the only other element present.
Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.
3.90/55.8 Fe : 1.1/16.0 O
=> 0.0700 Fe : 0.0.069 O
Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.
0.0700/0.069 Fe : 0.0700/0.0694 O
1 Fe : 1 O
Step 4 Multiply to remove any fractions
It is clear from the ratio that the numbers are whole numbers and hence this step is not necessary

FeO

6) A compound is found to contain 26.56% potassium, 35.41% chromium, and the remainder oxygen. Find its empirical formula.
Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.
26.56 g of K : 35.41g of Cr : 38.03 g of O
Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.
26.56/39.1K : 35.41/52.0 Cr of H : 38.03/16.0O
=> 0.68 K : 0.68 Cr : 2.4 O
Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.
Divide all by the lowest number of mol (0.68)
=> 0.68/0.68 K : 0.68/0.68 Cr : 2.4/0.68 O
1K:1Cr:3.5O
Step 4 Multiply to remove any fractions
It is clear from the ratio that the numbers are nowhere near whole numbers and hence we cannot simply round up or down. Here we have 3.5 mol of oxygen for every mol of K and Cr. We therefore remove the fraction by multiplying the entire ratio by 2.

$K_2Cr_2O_7$

7) A 60.00 g sample of tetraethyllead, a gasoline additive, is found to contain 38.43 g lead, 17.83 g carbon, and 3.74 g hydrogen. Find its empirical formula.

Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.

Since we are given masses we can skip this step

Step 2 Calculate the mol of each element present by dividing the mass of each element by its relative atomic mass.

38.43/207.2 Pb : 17.83/12.0 C : : 3.74/1.0 H

=> 0.185 Pb : 1.485 C : 3.74 H

Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.

=> 0.185/0.185 Pb : 1.485/0.185 C : 3.74/0.185 H

=>Pb : 8 C : 20H

Step 4 Multiply to remove any fractions

It is clear from the ratio that the numbers are whole numbers and hence this step is not necessary

PbC_8H_{20}

8) Determine the empirical formula for a compound with the following percent composition, by mass, 15.8% carbon and 84.2% sulphur.

Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.

15.8 g of C : 84.2 g of S

Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.

15.8 / 12.0 C : 84.2 / 32.1 S

=> 1.32 C : 2.62 S

Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.

Divide all by the lowest number of mol (1.32)

1.32/1.32 C : 2.62/1.32 S

=> 1 C: 2S

Step 4 Multiply to remove any fractions

Since there are no fractions and the mol of each element was close to a whole number, this step is not required.

CS_2

9) Determine the empirical formula for a compound with the following percent composition, by mass, 40.0% carbon, 6.7% hydrogen, and 53.3% oxygen.

Step 1 Find the mass of each element or convert the percentage composition into mass by assuming you have 100 grams of the compound.

40.0 g of C : 6.7 g of H : 53.3 g of O

Step 2 Calculate the mol of each element present by dividing each element by its relative atomic mass.

40.0 / 12.0 C : 6.7 / 1.0 H : 53.3 / 16.0 O

=> 3.33 C : 6.7 H : 3.33 O

Step 3 Find the simplest mol ratio of each element by dividing by the lowest number of mol.

Divide all by the lowest number of mol (3.33.0)

3.33/3.33 C : 6.7/3.33 H : 3.33/3.33 O

=> 1 C: 2 H : 1 O

Step 4 Multiply to remove any fractions

Since there are no fractions and the mol of each element was close to a whole number, this step is not required.

CH_2O

10) A 9.90 gram sample of pure *Polyvinylidene chloride*, from question 1b above, contains 0.100 mol of the pure substance. Give the molecular formula of *Polyvinylidene chloride.*

Step 1 Find the formula mass(F_m)

=> Use the formula

mol = mass/F_m

=> F_m =mass / mol = 9.90 / 0.100 = 99.0 amu.

Step 2 Starting from the empirical formula that was derived in question 1b find the number that the empirical formula must be multiplied by give the molecular formula.

=> let x be the number that the empirical formula must be multiplied by.

=> x = formula mass / empirical mass

=> = 99.0 / 49.5 = 2

Step 3 Find the molecular formula

=> CHCl X 2 = $C_2H_2Cl_2$