

EMPIRICAL FORMULA/MOLECULAR FORMULA

The **EMPIRICAL FORMULA** tells us the simplest formula and tells us the simplest whole number ratio of atoms. It also tells us the simplest mole ratio of elements in the compound.

The **MOLECULAR FORMULA** tells us the actual number of atoms of each element in a molecule or formula unit of a compound.

While the empirical and molecular formulae of a compound are sometimes the same, sometimes they are different.

Examples

COMPOUND	EMPIRICAL FORMULA (EF)	MOLECULAR FORMULA (MF)	MOLECULAR FORMULA IS ? TIMES LARGER THAN EF
carbon dioxide	CO ₂	CO ₂	MF = 1 x EF
phosphorous trisulfide	P ₂ S ₃	P ₂ S ₃	MF = 1 x EF
butane	C ₂ H ₅	C ₄ H ₁₀	MF = 2 x EF
phosphorous oxide	P ₂ O ₄	P ₄ O ₈	MF = 2 x EF
benzene	CH	C ₆ H ₆	MF = 6 x EF

CALCULATING EMPIRICAL FORMULAE:

In order to write the empirical formula of a compound we need to determine the simplest mole ratio in which the elements are combined.

Reminder: The number of moles, n , of an element may be calculated using the following formula.

$$n = m/M \text{ where } m = \text{given mass(g)} \text{ and } M \text{ is the molar mass (g/mol)}$$

Example: # moles in 0.407 g of magnesium: $n = \frac{0.407 \text{ g}}{24.3 \text{ g/mol}} = 0.0167 \text{ mol}$

Note that the units also are correct. $\frac{\text{g}}{\text{g/mol}} = \cancel{\text{g}} \times \frac{\text{mol}}{\cancel{\text{g}}} = \text{mol}$

Example #1: What is the empirical formula of a compound which has been found by quantitative analysis to contain 0.597 g carbon and 0.147 g hydrogen?

solution:

	mass (g)	#moles ($n = m/M$) $\frac{\text{g}}{\text{g/mol}} = \text{mol}$	actual mole ratio	whole # ratio	empirical formula
C	0.597	$\frac{0.597 \text{ g}}{12 \text{ g/mol}} = 0.0497 \text{ mol}$	$\frac{0.0497}{0.0497} = 1.00$	1	CH ₃
H	0.147	$\frac{0.147 \text{ g}}{1.01 \text{ g/mol}} = 0.146 \text{ mol}$	$\frac{0.146}{0.0497} = 2.93$	3	

Note: the actual mole ratio was not exactly a whole number. However 2.93 is close enough to 3 so we can round it off.

Example #2 - What is the empirical formula of a compound whose

percentage composition is found to be 69.9% iron and 30.1% oxygen?

- the key here is to assume that you are working with 100g of the compound

$$m_{\text{Fe}} = 69.9\% \times 100.0 \text{ g Fe} = 69.9 \text{ g}$$

$$M_{\text{Fe}} = 55.8 \text{ g/mol}$$

$$m_{\text{O}} = 30.1\% \times 100.0 \text{ g O} = 30.1 \text{ g}$$

$$M_{\text{O}} = 16.00 \text{ g/mol}$$

$$\begin{aligned} n_{\text{Fe}} &= 69.9 \text{ g} \times \frac{1 \text{ mol}}{55.80 \text{ g}} \\ &= 1.25 \text{ mol} \end{aligned}$$

$$\begin{aligned} n_{\text{O}} &= 30.1 \text{ g} \times \frac{1 \text{ mol}}{16.00 \text{ g}} \\ &= 1.88 \text{ mol} \end{aligned}$$

The molar ratio for Fe:O is 1.25:1.88. Dividing by 1.25 to obtain the lowest ratio, we obtain the molar ratio of Fe:O to be 1:1.5. Multiplying this ratio by 2, we obtain a final 2:3 ratio.

The empirical formula of the compound is Fe_2O_3 .

CALCULATING MOLECULAR FORMULAE

This 'whole number multiple' may be determined by comparing the molar mass (M) to the empirical formula mass (EMF). The following formula may be used.

$$MF = EF \times M/EMF$$

Suppose a compound with an empirical formula (EF) of CH₂O has a molar mass of 180 g. The molecular formula (MF) of this compound would be determined as follows:

$$MF = EF \times \frac{M}{EMF} = CH_2O \times \frac{180 \text{ g/mol}}{30 \text{ g/mol}} \leftarrow (EMF = 12 + 2(1) + 16 = 30 \text{ g/mol})$$

$$= (CH_2O) \times 6 = C_6H_{12}O_6$$

Example #1 Calculate the empirical formula and the molecular formula of a compound containing 3.215 g carbon, 0.357 g hydrogen and 1.428 g oxygen. The molar mass of the compound is 168 g/mol

Solution

element	mass (g)	# mol $n = m/M$	actual mol ratio	whole # ratio
C	3.215	$\frac{3.215\text{g}}{12.0 \text{ g/mol}} = 0.268 \text{ mol}$	$\frac{0.268 \text{ mol}}{0.0893 \text{ mol}} = 3.00$	3
H	0.357	$\frac{0.357\text{g}}{1.01 \text{ g/mol}} = 0.353 \text{ mol}$	$\frac{0.353 \text{ mol}}{0.0893 \text{ mol}} = 3.95$	4
O	1.428	$\frac{1.428\text{g}}{16.0 \text{ g/mol}} = 0.0893 \text{ mol}$	$\frac{0.0893 \text{ mol}}{0.0893 \text{ mol}} = 1.00$	1

The EF, empirical formula of this compound is C₃H₄O.

The mass of this, the EFM is 3(12) + 4(1) + 16 = 36 + 4 + 16 = 56 g

$$MF = EF \times \frac{M}{EFM} = (C_3H_4O) \times \frac{168 \text{ g/mol}}{56 \text{ g/mol}} = (C_3H_4O) \times 3 = C_9H_{12}O_3$$

∴ The molecular formula of the compound is C₉H₁₂O₃.

Example #2 - A compound was found to contain 10.06% C, 89.10% Cl, and 0.84% H, by mass. If the molar mass of the compound is 119.6 g/mol,

calculate its molecular formula.

Again, the key here is to assume that you are working with 100 g of the compound.

$$m_{\text{C}} = 10.06\% \times 100.0 \text{ g C} = 10.06 \text{ g}$$

$$M_{\text{C}} = 12.01 \text{ g/mol}$$

$$m_{\text{Cl}} = 89.10\% \times 100.0 \text{ g Cl} = 89.10 \text{ g}$$

$$M_{\text{Cl}} = 35.50 \text{ g/mol}$$

$$m_{\text{H}} = 0.84\% \times 100.0 \text{ g H} = 0.84 \text{ g}$$

$$M_{\text{H}} = 1.01 \text{ g/mol}$$

$$\begin{aligned} n_{\text{C}} &= 10.06 \text{ g} \times \frac{1 \text{ mol}}{12.01 \text{ g}} & n_{\text{Cl}} &= 89.10 \text{ g} \times \frac{1 \text{ mol}}{35.50 \text{ g}} & n_{\text{H}} &= 0.84 \text{ g} \times \frac{1 \text{ mol}}{1.01 \text{ g}} \\ &= 0.84 \text{ mol} & &= 2.51 \text{ mol} & &= 0.83 \text{ mol} \end{aligned}$$

The molar ratio for C:Cl:H is 0.84:2.51:0.83. Dividing by 0.83 to obtain the lowest ratio, we obtain the molar ratio of 1:3:1. The empirical formula of the compound is CCl_3H .

$$\begin{aligned} \text{empirical formula mass} &= 12.01 \text{ u} + (3 \times 35.50 \text{ u}) + 1.01 \text{ u} \\ &= 119.52 \text{ u} \end{aligned}$$

$$\begin{aligned} \frac{\text{molecular mass}}{\text{empirical formula mass}} &= \frac{119.6 \text{ u}}{119.52 \text{ u}} \\ &= 1 \end{aligned}$$

The molecular formula of the compound is CCl_3H .

Combustion Problems - Empirical/Molecular Formulae

When an organic compound undergoes complete combustion, the compound reacts with oxygen, and all the elements in the original compound are oxidized – with the exception of oxygen itself.

Thus

C (in the original compound) \rightarrow CO_{2(g)}

H (in the original compound) \rightarrow H₂O_(g)

S (in the original compound) \rightarrow SO_{2(g)}

N (in the original compound) \rightarrow NO_{2(g)}

- The mass of carbon in the CO_{2(g)} formed will be the same as the mass of C in the original compound (Law of Conservation of Mass), and it can be calculated as follows –

$$\text{mass of C in CO}_{2(g)} = (\text{mass of CO}_{2(g)} \text{ formed}) \times 12.0 \text{ g}/44.0 \text{ g}$$

- The mass of hydrogen in the H₂O_(g) formed will be the same as the mass of H in the original compound, and it can be calculated as follows –

$$\text{mass of H in H}_{2}\text{O}_{(g)} = (\text{mass of H}_{2}\text{O}_{(g)} \text{ formed}) \times 2.01 \text{ g}/18.0 \text{ g}$$

- Sulphur and nitrogen are calculated in a similar way
- It is not possible, however, to calculate the mass of oxygen present in the original compound in this manner, since the compound has taken in additional oxygen from the air. Instead, if the compound contains oxygen, its mass must be calculated by subtracting the sum of the masses of all the other elements from the mass of the compound.

Empirical & Molecular Formula Questions (additional practice)

1. The empirical formula of maleic acid is CHO. Its molecular mass is 116 g/mol. What is its molecular formula?
2. A well known reagent in analytical chemistry, dimethylglyoxime, has the empirical formula C_2H_4NO . If its molar mass is 116 g/mol, what is the molecular formula of the compound.
3. A compound contains C, H and O. A 5.000 g sample contains 3.215 g carbon and 0.357 g hydrogen. A gaseous sample of this gas has a mass 5.25 times the mass of an identical volume of oxygen gas under the same conditions. What is the molecular formula of the compound?
4. Cinnamic alcohol is used mainly in perfumery, particularly soaps and cosmetics. Its molecular formula is $C_9H_{10}O$.
 - (a) Calculate the percent composition by mass of C, H, and O in cinnamic alcohol.
 - (b) How many molecules of cinnamic alcohol are contained in a sample of mass 0.469g?
5. The molar mass of caffeine (ahhh.....sweet caffeine) is 194.19 g. Caffeine molecules are made up of C, H, N and O. If the empirical formula of caffeine is $C_4H_5N_2O$, what is the molecular formula?
6. Monosodium glutamate (MSG) has sometimes been suspected as the cause of “Chinese restaurant syndrome” because this food-flavour enhancer can induce headaches and chest pains. (interestingly, note that the Chinese people have used MSG for at least a thousand years with no ill effects). MSG has the following composition by mass –

35.51% C	4.77% H	37.85% O	8.29% N	13.60% Na
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 What is the molecular formula if its molar mass is 169 g?
8. A certain hydrocarbon is found to consist of 83.6% carbon and 16.4% hydrogen (by mass). If one molecule of this compound has a mass of 1.43×10^{-22} g, calculate its molecular formula.
10. When oleic acid is analysed it is found to consist of 76.6% carbon, 12.1% hydrogen and 11.3% oxygen (by mass). It is also found that there are exactly 18 times as many atoms present in one molecular of oleic acid than there are in one molecule of water! Calculate the molecular formula of oleic acid.