Composition of Compounds
Representing compounds Chemical formulas and molecular formulas

Determining Chemical formula form experimental data

### 3.7 Composition of Compounds

## Molar Mass of Compounds

- The relative masses of molecules can be calculated from atomic masses

Formula Mass = 1 molecule of $\mathrm{H}_{2} \mathrm{O}$
$=2(1.01 \mathrm{amu} \mathrm{H})+16.00 \mathrm{amu} \mathrm{O}=18.02 \mathrm{amu}$

- 1 mole of $\mathrm{H}_{2} \mathrm{O}$ contains 2 moles of H and 1 mole of O so molar mass = 1 mole $\mathrm{H}_{2} \mathrm{O}$
$=2(1.01 \mathrm{~g} \mathrm{H})+16.00 \mathrm{~g} \mathrm{O}=18.02 \mathrm{~g}$



## Percent Composition

- Percentage of each element in a compound $\checkmark$ by mass
نسبة العنصر في المركب
- Can be determined from

1. the formula of the compound
2. the experimental mass analysis of the compound

- The percentages may not always total to $100 \%$ due to rounding


## Percentage $=\frac{\text { part }}{\text { whole }} \times 100 \%$

## Example: Find the mass percent of Cl in $\mathrm{C}_{2} \mathrm{Cl}_{4} \mathrm{~F}_{2}$

| Given: Find: | $\begin{aligned} & \mathrm{C}_{2} \mathrm{Cl}_{4} \mathrm{~F}_{2} \\ & \% \mathrm{Cl} \text { by mass } \end{aligned}$ |
| :---: | :---: |
| Conceptual Plan: <br> Relationships: | $\begin{aligned} & \text { Mass } \% \mathrm{Cl}=\frac{4 \times \text { molar mass } \mathrm{Cl}^{\text {molar mass } \mathrm{C}_{2} \mathrm{Cl}_{4} \mathrm{~F}_{2}} \times 100 \%}{\text { Mass } \% \text { element } X=\frac{\text { mass element } X \text { in } 1 \mathrm{~mol}}{\text { mass } 1 \mathrm{~mol} \text { of compound }} \times 100 \%} \end{aligned}$ |
| $\begin{array}{r} \text { Solution: } \quad \begin{array}{r} 4 \times \text { molar mass } \mathrm{Cl}=4(35.45 \mathrm{~g} / \mathrm{mol})=141.8 \mathrm{~g} / \mathrm{mol} \\ \text { molar mass } \mathrm{C}_{2} \mathrm{Cl}_{4} \mathrm{~F}_{2}=2(12.01)+4(35.45)+2(19.00)=203.8 \mathrm{~g} / \mathrm{mol} \\ \text { Mass } \% \mathrm{Cl}=\frac{141.8 \mathrm{~g} / \mathrm{mol}}{203.8 \mathrm{~g} / \mathrm{mol}} \times 100 \%=69.58 \% \end{array} \end{array}$ |  |
| Check: | because the percentage is less than 100 and Cl is much heavier than the other atoms, the number makes sense |

Example 2 :Determine the mass percent composition of $\mathrm{CaCl}_{2}(\mathrm{Ca}=40.08, \mathrm{Cl}=35.45)$

- $\mathrm{CaCl}_{2} \quad$ Mass $\% \mathrm{Ca}=\frac{\text { molar mass } \mathrm{Ca}}{\text { molar mass } \mathrm{CaCl}_{2}} \times 100 \%$ Mass $\% \mathrm{CI}=\frac{2 \times \text { molar mass Cl }}{\text { molar mass } \mathrm{CaCl}_{2}} \times 100 \%$ $2 \times$ molar mass $\mathrm{Cl}=2(35.45 \mathrm{~g} / \mathrm{mol})=70.90 \mathrm{~g} / \mathrm{mol}$ molar mass $\mathrm{CaCl}_{2}=1(40.08)+2(35.45)=110.98 \mathrm{~g} / \mathrm{mol}$ Mass $\% \mathrm{Ca}=\frac{40.08 \mathrm{~g} / \mathrm{mol}}{110.98 \mathrm{~g} / \mathrm{mol}} \times 100 \%=36.11 \%$
Mass $\% \mathrm{Cl}=\frac{70.90 \mathrm{~g} / \mathrm{mol}}{110.98 \mathrm{~g} / \mathrm{mol}} \times 100 \%=63.88 \%$


### 3.8 Representing compounds Chemical formulas and molecular formulas

| Empirical <br> formula | Molecular <br> formula | Structural formula | Molecular <br> Models (3D) |
| :---: | :---: | :---: | :---: |
| HO | $\mathrm{H}_{2} \mathrm{O}_{2}$ | H-O-O-H |  |
| $\mathrm{CH}_{3}$ | $\mathrm{C}_{2} \mathrm{H}_{6}$ |  |  |

Empirical Formula - A formula that gives the simplest whole-number ratio of atoms in a compound.
هي الفورميولا او الصيغه التي تعطي اصغر نسب العناصر في المركب بالنسبه لبعضها

### 3.9 Steps for Determining an Empirical Formula

1. Start with the number of grams of each element, given in the problem.
2. ابدا بالوزن لكل عنصر في المساله المعطاه

- If percentages are given, assume that the total mass is 100 grams so that

$$
\text { اذا كان المعطاه نسبه مئويه, نفترض ان الوزن الكلي عباره عن } 100 \text { غم }
$$

the mass of each element $=$ the percent given.
كتله كل عنصر = النسبه المئويه المعطاه لكل عنصر
2. Convert the mass of each element to moles using the molar mass from the periodic table.
2. نقوم بتحويل كتلة كل عنصر الى مول وذلك بالاستعانه بالكتله الموليه المعطاة لكل عنصر بالجدول الدوري
3. Divide each mole value by the smallest number of moles calculated.

$$
\text { 3. نقسم كل قيمه موليه على اصغر قيمه من التي قد حسبت في نقطه } 2
$$

4. Then multiply each solution by the same factor to get the lowest whole number multiple

$$
\text { 4. ومن ثم نحاول ان تكون كل القيم التي حصبت في رقم } 3 \text { ان تكون عباره عن اعداد صحيحه }
$$

This is the mole ratio of the elements and is represented by subscripts in the empirical formula.
و هنا نكون قد وجدنا نسبه العناصر الى بعضها في المركب

## Example Problem \#1

A compound was analyzed حل and found to contain $13.5 \mathrm{~g} \mathrm{Ca}, 10.8 \mathrm{~g} \mathrm{O}$, and 0.675 g
H. What is the empirical formula of the compound?

Step 1
Start with the number of grams of each element, given in the problem.
Given $\downarrow$
13.5 g Ca
10.8 g O
0.675 g H

Step 2
Convert the mass of each element to moles using the molar mass from the periodic table.

Given $\downarrow \quad$ P.T. $\downarrow$
13.5 gea $\times \frac{1 \mathrm{~mol} \mathrm{Ca}}{40.1 \text { gea }}=0.337 \mathrm{~mol} \mathrm{Ca}$
$10.8 \mathrm{~g} \sigma \times \frac{1 \mathrm{molO}}{16.0 \mathrm{~g} \sigma}=0.675 \mathrm{~mol} \mathrm{O}$
$0.675 \mathrm{~g} \mathrm{HA} \times \frac{1 \mathrm{~mol} \mathrm{Ca}}{1.01 \mathrm{gHH}}=0.668 \mathrm{~mol} \mathrm{H}$
Step 3
Divide each mole value by the smallest number of moles calculated.

> Given $\downarrow \quad$ P.T. $\downarrow$
> $13.5 \mathrm{~g} \ell \mathrm{a} \times \frac{1 \mathrm{~mol} \mathrm{Ca}}{40.1 \mathrm{gCa}}=\frac{0.337}{0.337} \mathrm{~mol} \mathrm{Ca} \Rightarrow 1.00$
> $10.8 \mathrm{~g} \varnothing \times \frac{1 \mathrm{~mol} \mathrm{O}}{16.0 \mathrm{~g} \varnothing}=\frac{0.675}{0.337} \mathrm{molO} \Rightarrow 2.00$
> $0.675 \mathrm{~g} \mathrm{HF} \times \frac{1 \mathrm{~mol} \mathrm{Ca}}{1.01 \mathrm{ghH}}=\frac{0.668}{0.337} \mathrm{~mol} \mathrm{H} \Rightarrow 1.98 \approx 2.00$

Step 4
Is not needed her since i have only whole numbers
This is the mole ratio of the elements and is represented by subscripts in the empirical formula.

$$
\mathrm{CaO}_{2} \mathrm{H}_{2} \Rightarrow \mathrm{Ca}(\mathrm{OH})_{2}
$$

Example Problem \#2
A compound decomposed to $57.14 \% \mathrm{C}, 6.16 \% \mathrm{H}, 9.52 \% \mathrm{~N}$, and $27.18 \%$
O. Calculate the empirical formula of this compound

Step 1

If percentages are given, assume that the total mass is 100 grams so that the mass of each element $=$ the percent given.

Given $\downarrow$
57.14 g C
6.16 g H
9.52 g N
27.18 g O

Step 2
Convert the mass of each element to moles using the molar mass from the periodic table.

$$
\begin{aligned}
& \text { Given } \downarrow \quad \begin{array}{c}
\text { P.T. } \downarrow \\
57.14 \mathrm{gC} \times \frac{1 \mathrm{~mol} \mathrm{C}}{12.0 \mathrm{gC}}=4.76 \mathrm{~mol} \mathrm{C} \\
6.16 \mathrm{gHF} \times \frac{1 \mathrm{~mol} \mathrm{H}}{1.01 \mathrm{gH}}=6.10 \mathrm{~mol} \mathrm{H} \\
9.52 \mathrm{gAN} \times \frac{1 \mathrm{~mol} \mathrm{~N}}{14.0 \mathrm{gNf}}=0.68 \mathrm{~mol} \mathrm{~N} \\
27.18 \mathrm{~g} \emptyset \times \frac{1 \mathrm{~mol} \mathrm{O}}{16.0 \mathrm{~g} \emptyset}=1.70 \mathrm{~mol} \mathrm{O}
\end{array}
\end{aligned}
$$

Step 3
Divide each mole value by the smallest number of moles calculated.

$$
\begin{aligned}
& \text { Given } \downarrow \\
& 57.14 \mathrm{gC} \times \frac{1 \mathrm{~mol} \mathrm{C}}{12.0 \mathrm{gC}}=\frac{4.76}{0.68} \mathrm{~mol} \mathrm{C} \Rightarrow 7 \\
& 6.16 \mathrm{gHC} \times \frac{1 \mathrm{~mol} \mathrm{H}}{1.01 \mathrm{gHC}}=\frac{6.10}{0.68} \mathrm{~mol} \mathrm{H} \Rightarrow 8.97 \approx 9 \\
& 9.52 \mathrm{gAF} \times \frac{1 \mathrm{~mol} \mathrm{~N}}{14.0 \mathrm{gNC}}=\frac{0.68}{0.68} \mathrm{~mol} \mathrm{~N} \Rightarrow 1 \\
& 27.18 \mathrm{~g} \varnothing \mathrm{~g} \times \frac{1 \mathrm{molO}}{16.0 \mathrm{~g} \emptyset}=\frac{1.70}{0.68} \mathrm{~mol} \mathrm{O} \Rightarrow 2.5
\end{aligned}
$$

This is the mole ratio of the elements and is represented by subscripts in the empirical formula.

Step 4
multiply each solution by the same factor to get the lowest whole number multiple.

$$
\begin{aligned}
& \text { Given } \downarrow \quad \text { P.T. } \downarrow \\
& 57.14 \mathrm{gC} \times \frac{1 \mathrm{~mol} \mathrm{C}}{12.0 \mathrm{gC}}=\frac{4.76}{0.68} \mathrm{~mol} \mathrm{C} \Rightarrow 7(2)=14 \\
& 6.16 \mathrm{~g} \not \mathrm{Hf} \times \frac{1 \mathrm{~mol} \mathrm{H}}{1.01 \mathrm{gH}}=\frac{6.10}{0.68} \mathrm{~mol} \mathrm{H} \Rightarrow 8.97 \approx 9(2)=18 \\
& 9.52 \mathrm{~g} \times \mathbb{N} \times \frac{1 \mathrm{~mol} \mathrm{~N}}{14.0 \mathrm{gN}}=\frac{0.68}{0.68} \mathrm{~mol} \mathrm{~N} \Rightarrow 1(2)=2 \\
& 27.18 \mathrm{~g} \sigma \times \frac{1 \mathrm{molO}}{16.0 \mathrm{~g} \sigma}=\frac{1.70}{0.68} \mathrm{molO} \Rightarrow 2.5(2)=5
\end{aligned}
$$

## Empirical formula $=\mathrm{C}_{14} \mathrm{H}_{18} \mathrm{~N}_{2} \mathrm{O}_{5}$

## Finding molecular formula

Once the empirical formula is found, the molecular formula for a compound can be determined if the molar mass of the compound is known.

1. Simply calculate the mass of the empirical formula
2. احسب الكتله الموليه لل empirical formula
3. Divide the molar mass of the compound by the mass of the empirical formula to find the ratio between the molecular formula and the empirical formula.
4. اقسم الكتله الموليه للمركب المطلوب معرفه ال molecular formula على الكتله الموليه لل empirical formula

$$
\begin{aligned}
& \text { Molar Mass of compound }
\end{aligned}
$$

3. Multiply all the atoms (subscripts) by this ratio to find the molecular formula.

$$
\text { 3. قم بضرب كل الذرات بالمعامل الذي وجدته في خطوة } 2
$$

## Example Problem \#1

Calculate the molecular formula of compound has a molar mass of $294.30 \mathrm{~g} / \mathrm{mol}$ and its empirical formula is $\mathrm{C}_{14} \mathrm{H}_{18} \mathrm{~N}_{2} \mathrm{O}_{5}$.

Step 1
The molar mass of $\mathrm{C}_{14} \mathrm{H}_{18} \mathrm{~N}_{2} \mathrm{O}_{5}$
we can find the molecular formula by finding the mass of the empirical formula

$$
\begin{gathered}
\mathrm{C}_{14} \mathrm{H}_{18} \mathrm{~N}_{2} \mathrm{O}_{5}=14(12.0 \mathrm{~g})+18(1.01 \mathrm{~g})+2(14.0 \mathrm{~g})+5(16.0 \mathrm{~g})=294 \mathrm{~g} / \mathrm{mol} \\
\text { from P.T. } \longrightarrow \mathrm{C} \\
\mathrm{H}
\end{gathered} \mathrm{~N} \quad \mathrm{~N} \quad \mathrm{O}
$$

Step 2

$$
\frac{\text { molar mass }}{\text { empirical formula }}=\frac{294.30 \mathrm{~g} / \mathrm{mol}}{294 \mathrm{~g} / \mathrm{mol}} \approx 1
$$

Step 3

$$
\mathrm{C}_{14} \mathrm{H}_{18} \mathrm{~N}_{2} \mathrm{O}_{5} \quad \mathrm{X} \quad 1 \quad \rightarrow \mathrm{C}_{14} \mathrm{H}_{18} \mathrm{~N}_{2} \mathrm{O}_{5}
$$

The molecular formula is the empirical formula

## Example Problem \#2

The simplest formula for vitamin C is $\mathrm{C}_{3} \mathrm{H}_{4} \mathrm{O}_{3}$. Experimental data indicates that the molecular mass of vitamin C is about 180 . What is the molecular formula of vitamin C?

First, calculate the sum of the atomic masses for $\mathrm{C}_{3} \mathrm{H}_{4} \mathrm{O}_{3}$. Look up the atomic masses for the elements from the Periodic Table.
the sum of the atomic masses for $\mathrm{C}_{3} \mathrm{H}_{4} \mathrm{O}_{3}$ is:
$3(12.0)+4(1.0)+3(16.0)=88.0 \mathrm{~g} / \mathrm{mol}$
$n=180 / 88$
$n=2$
molecular formula vitamin $\mathrm{C}=2 \times \mathrm{C}_{3} \mathrm{H}_{4} \mathrm{O}_{3}=\mathrm{C}_{6} \mathrm{H}_{8} \mathrm{O}_{6}$

## MORE EXAMPLES

1 \# Determine the empirical formula and the molecular formula for a compound with the following elemental composition:

$$
40.00 \% \mathrm{C}, 6.72 \% \mathrm{H}, 53.29 \% \text { O. }
$$

The molecular weight of the compound was found to be $180 \mathrm{~g} / \mathrm{mol}$.

Solution:
The first step will be to assume exactly 100 g of this substance. This means in 100 g of this compound, 40.00 g will be due to carbon, 6.72 g will be due to hydrogen, and 53.29 g will be due to oxygen.

Then convert each of these masses to moles, using their respective atomic weights

$$
\begin{aligned}
& 40.00 \mathrm{~g} \mathrm{Cx} \frac{1 \mathrm{~mol} \mathrm{C}}{12.01 \mathrm{~g} \mathrm{C}}=3.331 \mathrm{~mol} \mathrm{C} \\
& 6.72 \mathrm{~g} \mathrm{Hx} \frac{1 \mathrm{~mol} \mathrm{H}}{1.008 \mathrm{~g} \mathrm{H}}=6.667 \mathrm{~mol} \mathrm{H} \\
& 53.29 \mathrm{~g} \mathrm{Ox} \frac{1 \mathrm{~mol} \mathrm{O}}{16.00 \mathrm{~g} \mathrm{O}}=3.331 \mathrm{molO}
\end{aligned}
$$

## Step 2

The smallest mole quantity is either the moles of carbon or moles of oxygen ( 3.331 mol )

$$
\begin{aligned}
& \frac{3.331 \mathrm{~mol} \mathrm{C}}{3.331 \mathrm{~mol}}=1.000 \mathrm{C}=1 \mathrm{C} \\
& \frac{6.667 \mathrm{~mol} \mathrm{H}}{3.331 \mathrm{~mol}}=2.001 \mathrm{H}=2 \mathrm{H} \\
& \frac{3.331 \mathrm{molO}}{3.331 \mathrm{~mol}}=1.0000=10
\end{aligned}
$$

Step 3
The ratio of $\mathrm{C}: \mathrm{H}: \mathrm{O}$ has been found to be 1:2:1, thus the empirical formula is: $\mathrm{CH}_{2} \mathrm{O}$.

Step 4
Calculate the molecular formula

$$
\frac{180 \mathrm{~g} / \mathrm{mol}}{30 \mathrm{~g} / \mathrm{mol}}=6
$$

The molecular formula is a multiple of 6 times the empirical formula:

$$
\mathrm{C}_{(1 \times 6)} \mathrm{H}_{(2 \times 6)} \mathrm{O}_{(1 \times 6)} \text { which becomes } \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}
$$

