

Empirical & Molecular Formulas

I. Percent Composition

1. Define the term percent composition.

Percent Composition - percent by mass of each element in a compound

2. Write out the formula for determining percent composition (by mass).

$$\text{Percent by Mass (element)} = \frac{\text{mass of element}}{\text{mass of compound}} \times 100$$

3. Determine the percent compositions of a 150-g sample of a compound that contains 85 g of Element X and 65 g of Element Y.

$$\begin{aligned} 1. \quad \frac{85 \text{ g element X}}{150 \text{ g compound}} \times 100 &= 56.7\% \\ 2. \quad \frac{65 \text{ g element Y}}{150 \text{ g compound}} \times 100 &= 43.3\% \end{aligned}$$

4. Write out the formula for determining percent composition (from the chemical formula).

$$\text{Percent by Mass (from formula)} = \frac{\text{mass of element}}{\text{molar mass of compound}} \times 100$$

5. Determine the percent by mass of NaHCO₃ (baking soda).

Step 1 : Determine molar masses of each element

$$\begin{array}{c|c|c|c} 1 \text{ mol Na} \times \frac{22.99 \text{ g Na}}{1 \text{ mol Na}} & 1 \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} & 1 \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} & 3 \text{ mol O} \times \frac{16.00 \text{ g O}}{1 \text{ mol O}} \\ \hline 22.99 \text{ g Na} & 1.008 \text{ g H} & 12.01 \text{ g C} & 48.00 \text{ g O} \\ \hline 84.01 \text{ g/mol} = (22.99 \text{ g Na}) + 1.008 \text{ g H} + 12.01 \text{ g C} + 48.00 \text{ g O} & & & \end{array}$$

Step 2 : Determine percent by mass of each element

$$\begin{array}{c|c|c|c} \frac{22.99 \text{ g/mol}}{84.01 \text{ g/mol}} \times 100 & \frac{1.008 \text{ g/mol}}{84.01 \text{ g/mol}} \times 100 & \frac{12.01 \text{ g/mol}}{84.01 \text{ g/mol}} \times 100 & \frac{48.00 \text{ g/mol}}{84.01 \text{ g/mol}} \times 100 \\ \hline 27.37 \% \text{ Na} & 1.200 \% \text{ H} & 14.30 \% \text{ C} & 57.14 \% \text{ O} \\ \hline \end{array}$$

II. Empirical & Molecular Formulas

1. Define the term empirical formula.

Empirical Formula - formula with the smallest whole-number mole ratio of the elements

2. Determine the mole ratio of a 150-g compound in which the percent composition is 40.05% sulfur (S) and 59.95% oxygen (O).

Step 1 : Determine the mass of each element.

$$\textcircled{1} \quad 150\text{g} \times .4005 = 60.07\text{g} \quad (\text{S})$$

$$\textcircled{2} \quad 150\text{g} \times .5995 = 89.93\text{g} \quad (\text{O})$$

Step 2 : Convert each element mass to moles.

$$\textcircled{1} \quad 60.07\text{g S} \times \frac{1\text{ mol S}}{32.07\text{g S}} = 1.873\text{ mol S}$$

$$\textcircled{2} \quad 89.93\text{g O} \times \frac{1\text{ mol O}}{16.00\text{g O}} = 5.621\text{ mol O}$$

Step 3 : Divide the moles of each element by the smallest number of moles.

$$\textcircled{1} \quad \frac{1.873\text{ mol S}}{1.873} = 1\text{ mol S}$$

$$\textcircled{2} \quad \frac{5.621\text{ mol O}}{1.873} = 3\text{ mol O}$$

Step 4 : Identify the empirical formula (based on ratios).



3. Define the term molecular formula.

Molecular Formula - the actual number of atoms of each element in one molecule (or formula unit) of the substance.

4. Benzene (liquid) and acetylene (gas) have similar percent compositions but different empirical formulas.

5. Write the equation to determine n (empirical formula multiplier) of a molecular formula.

$$n = \frac{\text{experimentally determined molar mass}}{\text{mass of empirical formula}}$$

6. Write the equation for determining molecular formula.

$$\text{Molecular Formula} = (\text{empirical formula}) n$$

7. If the Experimentally-Determined molar mass of benzene is 78.12 g/mol and acetylene is 26.04 g/mol, what is the molecular formula of each compound?

Acetylene
Benzene

$$\frac{26.04\text{ g/mol}}{13.02\text{ g/mol}} = 2.00$$



Benzene
Acetylene

$$\frac{78.12\text{ g/mol}}{13.02\text{ g/mol}} = 6.00$$



III. Hydrates

1. Define the term hydrate

Hydrate - Compound that has a specific number of water molecules bound to its atoms

2. Identify each hydrate name for each molecule of water bound.

Molecules	Hydrate Name	Molecules	Hydrate Name
1 =	mono hydrate	6 =	hexahydrate
2 =	dihydrate	7 =	heptahydrate
3 =	trihydrate	8 =	octahydrate
4 =	tetrahydrate	9 =	nona hydrate
5 =	penta hydrate	10 =	deca hydrate

3. Determine the hydrate formula of $\text{BaCl}_2 \cdot x\text{H}_2\text{O}$.

Step 1 : Find the difference between hydrate BaCl_2 (5.00 g) and anhydrous BaCl_2 (4.26 g).

$$5.00 \text{ g BaCl}_2 \text{ hydrate} - 4.26 \text{ g anhydrous BaCl}_2 = 0.74 \text{ g H}_2\text{O}$$

Step 2 : Convert BaCl_2 and H_2O to moles.

$$\textcircled{1} \quad 4.26 \text{ g BaCl}_2 \times \frac{1 \text{ mol BaCl}_2}{208.23 \text{ g BaCl}_2} = 0.0205 \text{ mol BaCl}_2$$

$$\textcircled{2} \quad 0.74 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} = 0.041 \text{ mol H}_2\text{O}$$

Step 3 : Calculate the ratio of H_2O to BaCl_2 .

$$x = \frac{0.041 \text{ mol H}_2\text{O}}{0.0205 \text{ mol BaCl}_2} = \frac{2}{1} \quad \text{BaCl}_2 \cdot 2\text{H}_2\text{O}$$

4. List uses for each of the following anhydrous or hydrate compounds.

Calcium chloride (anhydrous) : Dessicators (dry air container)

Calcium sulfate (anhydrous) : Ethanol additive (free from water)

Sodium sulfate (decahydrate) : Stores solar energy (when above 32°C)
(below 32°C → hydrate recrystallizer)