Pharmaceutical analytical chemistry I

- Lecture 4
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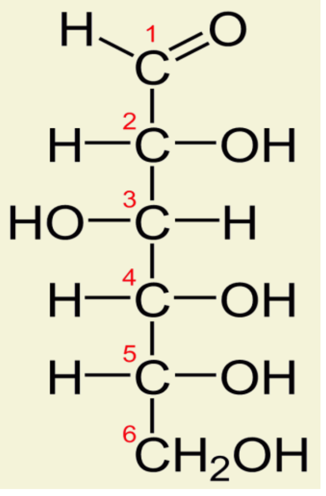
Representing Compounds: Chemical Formulas

Types of chemical formula

Molecular formula
- Formula that describes the number and types of atoms in a single molecule or compound e.g. molecular formula of glucose is $C_6H_{12}O_6$.

Empirical formula
- Formula that indicates simplest ratio of atoms in whole molecule e.g. empirical formula of glucose is $\mathbf{CH_2O}$.

Structural formula
- Formula that indicates the position of atoms in space (connectivity of atoms) e.g. structural formula of glucose



Structural formula of glucose

Example: Write empirical formulas for the compounds represented by the molecular

- formulas.
- **(a)** C_4H_8 **(b)** B_2H_6 **(c)** CCl_4

SOLUTION

- To determine the empirical formula from a molecular formula, *divide the subscripts by the greatest common factor* (the largest number that divides exactly into all of the subscripts):
- **(a)** For C_4H_8, the greatest common factor is 4. The empirical formula is therefore CH_2.
- **(b)** For B_2H_6, the greatest common factor is 2. The empirical formula is therefore BH_3.
- **(c)** For CCl_4, the only common factor is 1, so the empirical formula and the molecular formula are identical.

- **Homework:**

1- Select the structural formula for water.

(a) H¬O **(b)** H¬H

(c) H¬O¬H **(d)** H_2O

2- Write the empirical formula for the compounds represented by each molecular formula:

(a) C_5H_{12} **(b)** Hg_2Cl_2 **(c)** $C_2H_4O_2$

Determining a Molecular Formula from an Empirical Formula and Molar Mass

- General strategy:

- Calculate the empirical formula mass.
- Divide the molar mass by the empirical formula mass to find *n*.
- Multiply the empirical formula by *n* to obtain the molecular formula.

- Example: The empirical formula of butanedione is C_2H_3O, and its molar mass is 86.09 g/mol. Determine its molecular formula.

- Answer

- GIVEN: Empirical formula = C_2H_3O molar mass = 86.09 g/mol
- FIND: Molecular formula

1- Empirical formula molar mass = 2(12.01 g/mol) + 3(1.008 g/mol) + 16.00 g/mol = 43.04 g/mol

2- n =molar mass/ empirical formula molar mass =86.09 /43.04 = 2

3- Molecular formula = C_2H_3O x 2 = $C_4H_6O_2$

- **CHECK :** Check the answer by calculating the molar mass of the formula as follows:

4(12.01 g/mol) + 6(1.008 g/mol) + 2(16.00 g/mol) = 86.09 g/mol

➢The calculated molar mass is in agreement with the given molar mass.

Determine molecular formula for glyceraldehyde which as a molar mass of 90.05 g/mol and empirical formula CH_2O

- Answer

- GIVEN: Empirical formula = CH_2O molar mass = 90.08 g/mol
- FIND: Molecular formula

1- Empirical formula molar mass = 12.01 g/mol + 2(1.008 g/mol) + 16.00 g/mol = 30.02 g/mol

2- n =molar mass/ empirical formula molar mass =90.08 /30.02 = 3

3- Molecular formula = CH_2O x 3 = $C_3H_6O_3$

- **CHECK :** Check the answer by calculating the molar mass of the formula as follows:

3(12.01 g/mol) + 6(1.008 g/mol) + 3(16.00 g/mol) = 90.05 g/mol

➢The calculated molar mass is in agreement with the given molar mass.

Writing Formulas for Ionic Compounds

- When you write the formula of an ionic compound, note the following:

❑Ionic compounds always contain a positive cation and negative anion.

❑ In a chemical formula, the sum of the charges of the positive ions (cations) must equal the sum of the charges of the negative ions (anions).

❑The formula of an ionic compound reflects the smallest whole-number ratio of ions.

- Example:

1- Write the formula for the ionic compound composed of sodium and chlorine:

1- The compound contains Na^{+1} cation and Cl^{-1} anion

2- to form electrically neutral compound, its formula must be NaCl

(it must contain one Na^{+} cation for every one Cl^{-} anion).

2- Write the formula for the ionic compound composed of *calcium* and chlorine:

1- The compound contains Ca^{+2} cation and Cl^{-1} anion

2- to form electrically neutral compound, its formula must be $CaCl_2$

(it must contain one Ca^{+2} cation for every two Cl^{-} anion).

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In general , to write the formula of ionic compounds:

- ● ***If the charges* are numerically equal**, **then no subscripts are necessary**
- ● **If the charges on the cation and anion are numerically different, we apply the following rule to make formula electrically neutral:** ***subscript of cation is numerically equal to charge on anion, and subscript of anion is numerically equal to charge on cation.***

HOW TO: *Write Formulas for Ionic Compounds*	**Writing Formulas for Ionic Compounds** Write the formula for the ionic compound that forms between aluminum and oxygen.	**Writing Formulas for Ionic Compounds** Write the formula for the ionic compound that forms between calcium and oxygen.
1. Write the symbol for the metal cation and its charge followed by the symbol for the nonmetal anion and its charge.	Al^{3+} O^{2-}	Ca^{2+} O^{2-}
2. Adjust the subscript on each cation and anion to balance the overall charge.	Al^{3+} O^{2-} ↓ Al_2O_3	Ca^{2+} O^{2-} ↓ CaO
3. Check that the sum of the charges of the cations equals the sum of the charges of the anions.	cations: $2(3+) = 6+$ anions: $3(2-) = 6-$ The charges cancel.	cations: 2+ anions: 2− The charges cancel.

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Mole fraction:

The ratio of the number of moles of one component to the total number of moles of all components in the mixture solution .

- XA = number of mole of A / Total no of moles
- XB = nB / Total no of moles
- XC = nC / Total no of moles

Where XA + XB + XC =1

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- ➡ mole % = mole fraction x 100

Mole fraction:

- Example: If 23 gm of ethyl alcohol (molar mass 46gm\mol)is dissolved in 54 gm of water (molar mass 18gm\mol). Calculate the mole fraction of ethyl alcohol and water in solution.

- Answer:

No. of moles of solute (ethyl alcohol) $n_B = \frac{mass}{molar\ mass} = \frac{23}{46} = 0.5$ mole

No. moles of solvent (water) $n_A = \frac{mass}{molar\ mass} = \frac{54}{18} = 3$ mole.

Total no. moles = 3+ 0.5 = 3.5 mol

Mole fraction of solute (ethyl alcohol) $X_B = \frac{nB}{nA+nB} = \frac{0.5}{3.5} = 0.1429$

Mole fraction of solvent (water) $X_A = \frac{nA}{nA+nB} = \frac{3}{3.5} = 0.8571$

Solutions

- **Solutions** are defined as homogeneous mixtures of two or more pure substances.
- The **solvent** is the substance in which solute dissolves to produce a homogenous mixture.
- The **solute** is the substance that dissolves in a solvent to produce a homogenous mixture.
- When water is the solvent, the solution is called an **aqueous solution**.

Types of solutions

Solution type	State of solute	State of solvent	Example
Gaseous solution	Gas	Gas	Air
Liquid solution	**1-Gas** 2- Liquid **3-Solid**	**Liquid**	**1-Soda water (CO_2 in H_2O)** **2- Ethanol in H_2O** **3- Brine (NaCl in H_2O)**
Solid solution	**1-Gas** **2- Liquid** **3- Solid**	Solid	**H_2 in solid Pt** **Hg(l) in Ag(s)** **Alloys (Cu + Au) سبائك**

Concentration of solution

- The amount of solute dissolved in a given amount of solvent or dissolved in a given amount of solution.

Solution concentration

- **Dilute solution:** a solution has **a low** concentration of solute
- **Saturated solution:** a solution that contains **the maximum** amount of solute that can be dissolved into the solvent at a given temperature.
- **Supersaturated solution :** a solution can contain **more solute than normal** by raising the temperature of the solvent.

Methods for expressing the concentration: Example

I-Weight, Volume, and Weight-to-Volume Ratios

II- Molality

III-Molarity

IV- Normality:

V- Parts per million or parts per billion

Methods for expressing the concentration

I-Weight, Volume, and Weight-to-Volume Ratios

- All express concentration as units of solute presenting in 100 units of solution:

- 1- **Weight-to-volume percent (% w/v): weight of solute /100 ml solution**

- 2- **Volume percent (% v/v)** : **volume of solute / 100 mL solution**

- 3- **Weight percent (% w/w): gm solute / 100 g solution**

Methods for expressing the concentration

- 1- **Weight-to-volume percent (% w/v): weight of solute /100 ml solution**

$$\frac{weight}{volume}\% = \frac{weight\ of\ solute}{volume\ of\ solution} \times 100$$

Example 1, **:** A solution is prepared by dissolving 1.5 gm NH_4NO_3, mL in 100 ml water . What is **% w/v** of NH_4NO_3

W/V % = (1.5 / 100) x 100 = 1.5 % w/v

Methods for expressing the concentration

● 2- **Volume percent (% v/v)** : volume of solute / 100 mL solution

A solution of 5 % v/v MeOH/ H_2O contains 5 ml MeOH in 100 ml H_2O

$$\frac{volume}{volume}\% = \frac{volume\ of\ solute}{volume\ of\ solution}\times 100$$

Example 1: Determine % v/v of a solution made by combining 25 mL of ethanol with enough water to produce 200 mL of the solution.

% v/v = (25 ml ethanol / 200 ml water) x 100 = 12. 5 % v/v

Example 2: A solution is prepared by dissolving 60 mL of hydrogen peroxide in enough water to make 2000 mL of solution. Identify the concentration of hydrogen peroxide solution.

Solution

Volume of solute is 60 mL Volume of solution is 2000 mL

% v/v = volume of solute /volume of solution x 100 = (60 mL/ 2000mL)x 100 = 3 % v/v

Methods for expressing the concentration

● 3- **Weight percent (% w/w):** gm solute / 100 g solution

$$\frac{weight}{weight}\% = \frac{weight\ of\ solute}{weight\ of\ solution}\times 100$$

To determine the weight per cent of a solution, **divide the mass of solute by mass of the solution** (solute and solvent together) and multiply by 100 to obtain per cent.

Example Determine the weight / weight percent concentration of glucose made by combining 10 g glucose and 90 gm water

. 10 g glucose + 90 g H_2O = 100 g solution.

- % glucose (solute) = (10/100) x 100 = 10 %. w/w
- % Solvent (water) = (90/100) x 100 = 90 % w/w

II- Molality (m): Molal concentration:

It is the number of moles of solute per 1000 g (1kg) solvent.
Unit of molality : m or mol/Kg

- **no of moles n = $\frac{mass}{m-wt}$ (solute).**
- **Molality (m) = $\frac{mass}{m-wt}$ (solute)x $\frac{1Kg}{W\ (solvent) in\ Kg}$**

N.B:
- W $_{solution}$ = W $_{solute}$ + W $_{solvent}$
- W $_{solvent}$ = W $_{solution}$ – W $_{solute}$
- W $_{solvent}$ = d V $_{solution}$ – W $_{solute}$
- Density (d) = mass/ volume

Where:
d = density of the solution
V = Volume of the solution

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II- Molality (m)

Example 1: What is the molality of 12.5 % solution of glucose $C_6H_{12}O_6$, in water? Molecular weight (M.wt.) or molar mass of glucose is 180.0

Solution:

1) 12.5 % solution means : 12.5 g $C_6H_{12}O_6$ is dissolved in 100 g solution.
W of solvent (water) = 100 – 12.5 = 87.5 g H_2O = 0.087 Kg H_2O

2) no. of moles glucose = mass / molar mass = 12.5/180

$$\text{Molality (m)} = \frac{mass}{molar\ mass}\text{(solute)x}\frac{1Kg}{W\ (solvent)}$$

$$\text{Molality (m)} = \frac{mass}{molar\ mass}\text{(solute)x}\frac{1\ Kg}{W\ (solvent)}$$

3) Molality (m) $= \frac{12.5}{180} \times \frac{1\ Kg}{0.087}$ = 0.794 m or 0.794 mol/ Kg

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III- Molarity (M):

The no. of moles of solute dissolved in 1 liter of solution.
M = No. of moles of solute per volume of solution in liter
Unit of molarity: M or mol/L

$$\textbf{Molarity (M)} = \frac{mass}{molar\ mass}\ \textbf{(solute) x} \left(\frac{1L}{V\ (soln.)}\right)$$

III- Molarity (M):

Example: NaCl ⟶ Na^+ + Cl^-

Dissolving 0.1 mole of NaCl in 1L of water gives a solution containing **0.1 moles of Na^+ and 0.1 moles of Cl^-**

Example: $CaCl_2$ ⟶ Ca^{2+} + 2 Cl^-

Dissolving 0.1 moles of $CaCl_2$ in 1 L of water gives a solution containing **0.1 moles of Ca^{2+} and 0.2 moles of Cl^-**

A square brackets [ ] around a species indicates that we are referring to molar concentration

Thus, $[Na^+]$ is read as "molar concentration of sodium ions".

III- Molarity (M):

Example: if 10.0 g of KCl is dissolved in 1000g of water . If the density of the solution is 0.997 g/ml . Calculate the molarity of the solution

Given that atomic masses of K = 39, Cl = 35.5

Solution:

Molar mass of KCl = 1 x 39 (K) + 1 x 35.5 (Cl) = 74.5 g/mole

Number of mole of solute = mass / molar mass

Mass of solution = mass of solute + mass of solvent = 10 + 1000 = 1010 g

Volume of solution = mass/ density = 1010 g /0.997 g/ml = 1013 ml = 1.013 L

$$M = \frac{mass}{molar\ mass} \times \left(\frac{1L}{V}\right) = \frac{10g}{74.5\ g/mole} \times \left(\frac{1}{1.013}L\right)$$

= 0.1342 mol/ 1.013L = 0.1325 mol/L or 0.1352 M

What is the difference between molarity and molality?

Molarity = mole of solute/ L of solvent

Molality = mole of solute/ Kg of solvent

- **Molality** is used in thermodynamic calculations . **Why ?**

- **Molarity is based on volume of solution containing solute.**
- **since volume of solution is affected by temperature → then its molar concentration changes with temperature.**
- **Therefore we should use solvent's mass in place of solution's volume, → so resulting concentration becomes independent of temperature.**
- **Accordingly in thermodynamic calculations we should use molality instead of molarity**

IV- Normality (N): is an equivalent concentration

Normal solution (N): Gram equivalent weight of solute (substance) in one liter of solution

- 1- Equivalent weight of acids or bases=

Molecular weight of acid or base / number of replacable H^+ or OH^-

Substance	No. of H^+ or OH^-	Equivalent weight
HCl	1	M.wt/1
NaOH	1	M.wt/1
H_2SO_4	2	M.wt/2
$Ca(OH)_2$	2	M.wt/2
H_3PO_4	3	M.wt/3
CH_3COOH	1	M.wt/1

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IV- Normality (N)

2- Equivalent weight of salts=

Molecular weight of salt / number of single atom x its valency

Substance	No. of single atom × valence	Equivalent weight
NaCl	1×1	M.wt/1
$CaCl_2$	1×2	M.wt/2
$AlCl_3$	3×1	M.wt/3
$Al_2(SO_4)_3$	3×2	M.wt/6

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IV- Normality (N)

Normality (N): number of equivalents in one liter of solution.
Normality= no. of equivalents/Volume (L)

Since No. of equivalents = weight (g)/equivalent weight

Normality (N)= $\dfrac{\textbf{weight (g)}}{\textbf{equivalent weight} \times \textbf{volume (L)}}$

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IV- Normality (N)

What is the normality of a solution containing 35 g of $MnCl_2.4\,H_2O$ in 300 ml of solution? (Mn= 55, Cl=35.5, H=1, O=16)

Molecular weight of $MnCl_2.4\,H_2O$ = 55 + 71 + 72 = 198

Equivelant weight= molecular weight/2=198/2=99

Normality= $\dfrac{\text{weight (g)}}{\text{equivalent weight} \times \text{volume (L)}} = \dfrac{35}{99x0.3} =$ **1.18 N.**

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V- Parts Per Million and Parts Per Billion

Trace concentrations are usually expressed in smaller units as

- **parts per million (ppm)** (one part in 10^{6})
- **or parts per billion** (ppb), (one part in 10^{9})

Commonly used are

ppm (parts-per-million, 10^{-6}),
ppb (parts-per-billion, 10^{-9}),
ppt (parts-per-trillion, 10^{-12})
and **ppq** (parts-per-quadrillion, 10^{-15})

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