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Module: Biophysics

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CHAPTER 2: General Information on Aqueous Solutions

1-Study of Solutions

A solution is a mixture of two or more substances, consisting of:

- Solvent: the substance present in the greatest amount.
- Solute: the substance(s) present in a smaller amount.

SOLUTION = SOLUTE + SOLVENT (homogeneous mixture, a single phase)

- Aqueous solution: A solution in which water is the solvent. Water molecules surround the solute molecules.

1-1-Degree of Dissociation:

It is the ratio of the number of moles of solute molecules that have dissociated to the initial number of moles of molecules. It is a dimensionless number:

$\alpha=1$ for a strong electrolytic solution

$\alpha<1$ for a weak electrolytic solution

$\alpha=0$: No dissociation

2-Concentrations:

A solution is characterized by the following parameters:

2-1 Mole Fraction:

The mole fraction is equal to the ratio of the number of moles of the solute to the total number of moles in the mixture of solute and solvent.

$$f_1=\frac{n1}{n1+n2} \quad , \quad f_2=\frac{n2}{n1+n2}$$

n_1: Number of molecules of one component.

n_2: Number of molecules of the other component.

F_1 and f_2 Unitless.

We see that $f_1+f_2=1$ If there are multiple components, the mole fraction of the i-th component is:

$$f_i=\frac{ni}{n1+n2+\cdots+ni+\cdots+np}$$

Exercise:

Determine the mole fraction of the solute and then that of the solvent in a 5% glucose serum.

Solution:

The composition of the solution is:

5 g of glucose (solute)

100 ml of water (solvent)

The solvent represents a quantity of substance of:

$n_{water}=\frac{100}{18}=5.555$ mol

The quantity of substance dissolved as solute is:

$n_{glucose}=\frac{5}{180}=0.027$ mol

The mole fractions are therefore:

Mole fraction of glucose:

$F_{glucose}=\frac{nglucose}{nwate+nglucose}=0.0048=0.48\%$

Mole fraction of water:

$F_{water}=\frac{nwater}{nwater+nglucose}=0.9952=99.52\%$

2-2- Weight Concentration (Mass Concentration)

Weight concentration, also known as mass concentration, is the ratio of the mass of the solute ms to the volume of the solution Vsol. It indicates how much solute is present in a given volume of the solution.

$Cp=\frac{m_s}{V_{sol}}$

Where:

- Cp is the weight concentration (in units such as (g/L) or (g/cm^3)).
- m_s is the mass of the solute.
- V_{solution} is the volume of the solution.

If the solvent is water at room temperature, then the two expressions are equivalent since 1L weighs approximately 1 kg

2-3 Molarity

The molar concentration of a given solute is the number of moles of the solute per liter of solution, given by:

$$\boldsymbol{C^M = \frac{n_{solute}}{v_{solution}}}$$

<u>Units:</u>

(number of moles): measured in moles (mol).

V (volume of the solution): measured in liters (L).

C^M (molar mass): measured in grams per mole (mol/L).

2-4 Molality

Molal concentration, or molality, is defined as the number of moles of solute per unit mass of solvent. It is expressed as:

$$\boldsymbol{C^m = \frac{n_{solute}}{m_{solvent}}}$$

<u>Units:</u>

n (number of moles): measured in moles (mol).

(mass of the solvent): measured in kilograms (kg).

C^m (molal concentration or molality): measured in moles per kilogram (mol/kg).

2-5 Ionic Concentration (Ionarity)

The concentration of ions in a solution can be determined using the following formula:

$[\text{ions}]=\alpha \cdot \upsilon_{\text{ions}} \cdot C^M$

α is the dissociation coefficient

υ_{ions} It is the number of ions produced by each molecule upon dissociation.

<u>Units:</u>

[ions]in ion g/l

Example:

$NaCl \longrightarrow Na^{+} + Cl^{-}$ $\upsilon_{Na^+} = 1$ $\upsilon_{Cl-} = 1$

$CaCl_2 \longrightarrow Ca^{++} + 2\,Cl^{-}$ $\upsilon_{Ca^{++}} = 1$ $\upsilon_{Cl^-} = 2$

2-6 Equivalent Concentration

For an ion i with an ionic concentration $[i]$ and valence , we have:

$$C_i^{eq} = |z_i| \ [i] = |z_i| \ \alpha\, \upsilon_i\, C^M$$

υ_i It is the number of ions produced by each molecule upon dissociation.

$|z_i|$ Electrovalence of the Solute Molecule

α: Dissociation Coefficient of the solute in the considered solvent.

Z^+ and Z^-: Valences of the ions.

+: Cation

−: Anion

Units:

C in eq g/l

Example:

Given that, the molar concentration of $CaCl_2$ is 2mol/L with a dissociation coefficient

α=1. Calculate the equivalent concentration of positive and negative ions. What can be concluded?

$CaCl_2 \longrightarrow Ca^{++} + 2\,Cl^{-}$ avec $\upsilon_{Ca++} = 1$ $\upsilon_{cl-} = 2$

$$C_{ca++}^{eq} = |z_{ca++}| \ [Ca^{++}] = |z_{ca++}| \ \alpha \ \upsilon_{Ca++} \ C^M = 2 \text{ x}1\text{x}1\text{x}2 = 4 \text{ Eqg /l}$$

$$C_{cl-}^{eq} = |z_{cl-}| \ [cl^{-1}] = |z_{cl-}| \ \alpha\, \upsilon_{cl-} \ C^M = 1\text{x}1\text{x}2\text{x}2 = 4 \text{ Eqg /l}$$

We note that the equivalent concentration of positive ions is always equal to the equivalent concentration of negative ions. Consequently, we have:

$C^{eq}{}_{+} = C^{eq}{}_{-}$

The total equivalent concentration of the solution, C^{eq}_{total}, will be the sum of the equivalent concentrations of the positive and negative ions.

2-7 Osmolar concentration or osmolarity C 0

Osmolarity is defined as the number of osmoles 'molecules and ions' dissolved per liter of solution.

$$C^{o} = (1 + \alpha(\upsilon - 1))\, C^{M}$$

$$C^{o} = i\, C^{M}$$

With

$i = 1 + \alpha(\upsilon - 1)$

“i” is called the van 't Hoff ionization coefficient.

Unit: C^0 in osmol.L^{-1}

2-8 Ionic strength of a solution

"Ionic strength of a solution" refers to a measure of the total concentration of ions in that solution. It helps to quantify how the presence of various ions affects properties like solubility and reaction rates. The formula for calculating ionic strength (μ) is:

$$\mu = \frac{1}{2}\left[\sum_i z_i^2 [i]\right]$$

μ: ionic strength,

[i]: ionic concentration of ion i in ion g/l

zi: valence of ion i.

Example: We take 1 mole of $CaCl_2$ with 2 moles of NaCl in a volume of 1 liter.

Calculate the ionic strength of the solution.

$z_{Ca^{++}} = +2$ et $z_{Cl^-} = -1$

$[Ca^{++}] = \upsilon_{Ca++}\ \alpha\ C^M = 1x1x1 = 1$ ion g/l

$[Na^+] = \upsilon_{Na+}\ \alpha\ C^M = 1x1x2 = 2$ ion g/l

$[Cl^-]_{NaCl} = \upsilon_{Cl-}\ \alpha\ C^M = 1x1x2 = 2$ ion g/l

$[Cl^-]_{CaCl2} = \upsilon_{Cl-}\ \alpha\ C^M = 2x1x1 = 2$ ion g/l

$$\mu = \frac{1}{2}\left[\ z^2_{Na+}[Na^+] + z^2_{cl-}[Cl^-] + z^2_{Ca++}[Ca^{++}] + z^2_{cl-}[Cl^-]\right]$$

$$= \frac{1}{2}[(1)^2 2+(1)^2.2+(2)^2.1+(-1)^2(2)]$$

$$= \frac{1}{2}[2+2+4+2]=5$$

3-Solubility

Solubility is the maximum amount of a substance that can dissolve in a given volume of water. The solubility of a pure substance depends, at a given temperature, on the structure of the compound and the nature of the solvent. To define the solubility product for a saturated solution (which is, by definition, a solution in dynamic equilibrium with undissolved solute), we define an equilibrium constant that is related to the solubility constant.

3-1The Equilibrium Constant

- For a weak binary electrolyte of the type AB

$$\mathbf{AB \rightleftharpoons A^+ + B^-}$$

The equilibrium constant k defined by:

$$k = \frac{[A^+].[B^-]}{[AB]} = \frac{\alpha^2 C_M}{1-\alpha}$$

- For a weak binary electrolyte of the type AB_2

$$\mathbf{AB_2 \Leftrightarrow A^{2+} + 2\ B^-}$$

In this case, the equilibrium constant $k$is equal to:

$$k = \frac{[A^+].[B^-]^2}{[AB]} = \frac{4\alpha^3 C_M{}^2}{1-\alpha}$$

4- Electrical properties of electrolytes

4-1 Electrical conductivity

Aqueous ionic solutions can conduct electricity (as conductors) because the Coulombic attraction diminishes, leading to an increased distance between ions, which weakens the bonds and results in either complete or partial dissolution of the crystal. In contrast, substances like pure water, oil, and glucose or urea solutions conduct very little to no electric current, as these are neutral solutions. The electrical resistance **R** of an electrolytic solution with resistivity $\boldsymbol{\rho}$, located in a container of length $\boldsymbol{l}$ and cross-section $\boldsymbol{S}$, is expressed as follows:

$$\boldsymbol{R = \frac{\rho . l}{S}}$$

R is in ohms,

ρ in ohm m,

l is the length of the container in m, and S is in m^2.

Electrical conductivity χ is expressed in $ohm^{-1}m^{-1}$ and is the inverse of resistivity; hence, the expression for conductivity is:

$$\chi = \frac{1}{\rho}$$