

Important Formulas of Physical Chemistry

THE SOLID STATE

1. Calculation of number of particles / atoms / ions in a Unit Cell :

2.	Type of Unit Cell	Numer of particles per Unit Cell	Relationship between edge length (a) and radius (r) of atom/ion
	Simple cubic	1	$a = 2r$
	Body centred cubic	2	$a = \frac{4}{\sqrt{3}} r$
	Face centred cubic	4	$a = 2\sqrt{2} r$

3. Density of unit cell (d)

$$d = \frac{Z \times M}{a^3 \times N_A}$$

Where **Z** is rank of unit cell (no. of atoms per unit cell), **m** is molar mass/ atomic mass, 'a' is edge length of the cube, 'a³' is volume of cubic unit cell and **N_A** is Avogadro number.

$$4. \text{ Packing efficiency} = \frac{d \times N_A}{M} \times \frac{4}{3} \pi r^3 \times 100$$

Here 'M' is molar mass 'r' is radius of atom, 'd' is density and **N_A** is Avogadro's number ($6.022 \times 10^{23} \text{ mol}^{-1}$).

Rank of unit cell can be computed by packing efficiency value

Type of Unit Cell	Packing efficiency	Rank of Unit Cell
SC	52.4%	1
BCC	68.0%	2
FCC	74%	4

Solution

1. Mole fraction (x)

if the number of moles of A and B are n_A and n_B respectively, the mole fraction of A and B will be

$$x_A = \frac{n_A}{n_A + n_B}, \text{ and } x_B = \frac{n_B}{n_A + n_B}$$

$$x_A + x_B = 1$$

2. **Molarity (M)** = $\frac{\text{Moles of solute}}{\text{Volume of solution in litres}}$

3. **Moality (m)** = $\frac{\text{Moles of solute}}{\text{Mass of solvent in kilograms}}$

4. Parts per million (ppm)

$$= \frac{\text{Number of parts of the component}}{\text{Total number of parts of all components of the solution}} \times 10^6$$

5. Raoult's law for a solution of volatile solute in volatile solvent :

$$p_A = p_A^\circ x_A$$

$$p_B = p_B^\circ x_B$$

Where p_A and p_B are partial vapour pressures of component 'A' and component 'B' in solution. p_A° and p_B° are vapour pressures of pure components 'A' and 'B' respectively.

6. Raoult's law for a solution of non-volatile solute and volatile solvent :

$$\frac{p_A^\circ - p_A}{p_A^\circ} = i x_B \approx i \frac{n_B}{N_A} = i \frac{W_B \times M_A}{M_B \times W_A} \text{ (for dilute solution)}$$

Where x_B is mole fraction of solute, i is van't Hoff factor and $\frac{p_A^\circ - p_A}{p_A^\circ}$ is relative lowering of vapour pressure.

7. **Elevation in boiling point (ΔT_b)**

$$\Delta T_b = i \cdot K_b \cdot m$$

where $\Delta T_b = T_b - T_b^\circ$

K_b = molal boiling point elevation constant

m = molality of solution.

8. **Depression in freezing point (ΔT_f)**

$$\Delta T_f = i \cdot K_f \cdot m$$

where $\Delta T_f = T_f^\circ - T_f$

K_f = molal depression constant

m = molality of solution.

9. **Osmotic pressure (π) of a solution**

$$\pi V = inRT \quad \text{or} \quad \pi = i CRT$$

where π = osmotic pressure in bar or atm

V = volume in litres

i = Van't Hoff factor

c = molar concentration in moles per litres

n = number of moles

T = Temperature on Kelvin Scale

$R = 0.083 \text{ L bar mol}^{-1} \text{ K}^{-1}$

$R = 0.0821 \text{ L atm mol}^{-1} \text{ K}^{-1}$

10. **Van't Hoff factor (i)**

$$i = \frac{\text{Observed colligative property}}{\text{Theoretically calculated colligative property}}$$

$$i = \frac{\text{Normal molar mass}}{\text{Abnormal molar mass}}$$

$$\begin{cases} i > 1 & \text{For dissociation of molecules} \\ i < 1 & \text{For association of molecules} \\ i = 1 & \text{For ideal solution} \end{cases}$$

11. **Relationship between relative lowering in vapour pressure and elevation in b.p.**

$$\frac{\Delta p}{p_A^\circ} = i \frac{\Delta T_b}{K_b} M_A \times 1000$$

Here

Δp is lowering in vapour pressure, p_A° is vapour pressure of pure solvent, i is van't Hoff factor, ΔT_b is elevation in boiling point, K_b is molal elevation constant and M_A is molar mass of solvent

Electrochemistry

1. **Conductivity (k)**

$$K = \frac{1}{P} = \frac{1}{R} \times \frac{l}{A} = G \times G^*$$

Where R is resistance, $l/A =$ cell constant (G^*) and $\frac{1}{P}$ is resistivity.

2. Relationship between k and Λ_m

$$\Lambda_m = \frac{1000 \times k}{c}$$

Where Λ_m is molar conductance, k is conductivity and C is molar concentration.

Kohlrausch's law

- (a) In general if an electrolyte on dissociation gives v_+ cations and γ_- anions then, its limiting molar conductivity is given by

$$\Lambda_m^\circ = \gamma_+ \lambda_+^\circ + \gamma_- \lambda_-^\circ$$

Here λ_+° and λ_-° are the limiting molar conductivities of cation and anion respectively and v_+ and v_- are the number of cations and anions furnished by one formula unit.

(b) **Degree of dissociation (α)** is given by :

$$\alpha = \frac{\Lambda_m^c}{\Lambda_m^\circ}$$

Here Λ_m° is molar conductivity at the concentration C and Λ_m° is limiting molar conductivity of the electrolyte.

(c) Dissociation constant (K.) of weak electrolyte

$$K = \frac{C\alpha^2}{1-\alpha} = \frac{C \left(\frac{\Lambda_m^c}{\Lambda_m^\circ} \right)^2}{\left(1 - \frac{\Lambda_m^c}{\Lambda_m^\circ} \right)}$$

3. **Nernst Equation for electrode reaction** : $M^{n+} + ne^- \rightarrow M$.

$$E = E^\theta - \frac{2.303 RT}{nF} \log \frac{1}{[M^{n+}]}$$

For Cell potential of electrochemical reaction $aA : bB \xrightarrow{ne^-} cC + dD$

$$E_{\text{cell}} = E_{\text{cell}}^\theta - \frac{2.303RT}{nF} \log [Q_c]$$

4. **Relationship between E^θ cell and equilibrium constant (K_c)**

$$E^\theta_{\text{cell}} = \frac{2.303RT}{nF} \log K_c$$

$$E^\theta_{\text{cell}} = \frac{0.059V}{n} \log K_c$$

5. $\Delta G^\theta = - nF E^\theta_{\text{cell}}$

Where ΔG^θ = standard Gibbs energy change and nF is the amount of charge passed.

$$\Delta G^\theta = - 2.303 RT \log K_c$$

Chemical Kinetics

1. Integrated rate law equation for zero order reaction

$$(a) \quad k = \frac{[R]_0 - [R]}{t}$$

Where k is rate constant and $[R]_0$ is initial molar concentration.

$$(b) \quad t_{1/2} = \frac{[R]_0}{2k}$$

$t_{1/2}$ is half life period of zero order reaction.

2. Integrated rate law equation for first order reaction

$$(a) \quad k = \frac{2.303}{t} \log \frac{[R]_0}{[R]}$$

Where k is rate constant, $[R]_0$ is initial molar concentration and $[R]$ is final concentration at time 't'.

(b) Half life period ($t_{1/2}$) for first order reaction :

$$t_{1/2} = \frac{0.693}{k}$$

3. Arrhenius equation

$$(a) \quad k = A e^{-E_a/RT}$$

Where 'A' is frequency factor, E_a is the energy of activation, R is universal gas constant and T is absolute temperature.

$e^{-E_a/RT}$ gives the fraction of collisions having energy equal to or greater than E_a .

$$(b) \quad \log \frac{k_2}{k_1} = \frac{E_a}{2.303 R} \left(\frac{T_2 - T_1}{T_1 T_2} \right)$$

Where k_1 is rate constant at temperature T_1 and k_2 is rate constant at temperature T_2 .