Important Formulas of Physical Chemistry

THE SOLID STATE

1. **Calculation of numer 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	$a = \dfrac{4}{\sqrt{3}} r$
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 Avogatro number.

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

Here 'M' is molar mass 'r' is radius of atom, 'd' is density and N_A is Avogaotro's number (6.022×10^{23} 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.%	2
FCC	74%	4

Solution

1. **Mole fraction (x)**

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

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

   $$x_A + x_B = 1$$

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

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

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. **Raoults law for a solution of non-volatile solute and volatile solvent :**

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

   Where x_B is mole fraction of solute, i is van't Hoff factor and $\dfrac{p_A^\circ - p_A}{p_A^\circ}$ is

   relative lowering of vapour pressure.

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

$$\Delta T_b = i.K_b\, m$$

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)**

$$\Delta T_f = i.K_f\, m$$

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**

$$\pi V = inRT \quad or \quad \pi = i\, CRT$$

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 L bar mol^{-1} K^{-1}

         R = 0.0821 L atm mol^{-1} 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 prescure 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, $p_A{}^\circ$ 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 ν_+ cations and γ_- anions then, its limiting molar conductivity is given by

$$\Lambda^\circ{}_m = \gamma_+ \, \lambda^\circ{}_+ + \gamma_- \, \lambda^\circ{}_-$$

Here $\lambda_+{}^\circ$ and $\lambda^\circ{}_-$ are the limiting molar conductivities of cation and anion respectively and ν_+ and ν_- 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^c is molar conductivity at the concentration C and Λ_m° is limiting molar conductivity of the electrolyte.

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

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

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 $aA : bB \xrightarrow{\ ne^-\ } cC + dD$

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

4. **Relationship between E° cell and equilibrium constant (Kc)**

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

$$E^\theta\ cell = \frac{0.059v}{n}\ \log\ K_c$$

5. $\Delta G^\theta = -\ nF\ E^\theta cell$

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) $k = \dfrac{[R]_\circ - [R]}{t}$

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

   (b) $t_{\frac{1}{2}} = \dfrac{[R]_\circ}{2k}$

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

2. **Integrated rate law equation for first order reaction**

   (a) $k = \dfrac{2.303}{t} \log \dfrac{[R]_\circ}{[R]}$

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

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

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

3. **Anhenius epuation**

   (a) $k = A \, e^{-Ea/RT}$

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

   $-Ea/_{RT}$ gives the fraction of collisions having energy equal to or greater than Ea.

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

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