Fundamentals of Distribution Separations (II)
(08/26/13)

1. Principles of distribution equilibria

$$dG = -S_* \, dT + V_* \, dP + \Sigma(\mu_i^{int} + \mu_i^{ext})dn_i$$ *(open systems under external field)*

$$K = \exp\left(\frac{-\Delta\mu_i^0 - \Delta\mu_i^{ext}}{RT}\right)$$ *distribution coefficient*

$$\Delta\mu_i^0 = \Delta\bar{H}_i^0 - T\Delta\bar{S}_i^0$$

$$\mathbf{A{-}{-}{-}B} \xrightarrow{q} \mathbf{A + B}$$

2. Intermolecular interactions

Intermolecular Interactions

Intermolecular interactions:

Dissociation of H_2O = 200 kcal/mol ($H_2O \longrightarrow 2\ H + O$)
Vaporization energy of H_2O = 9.7 kcal/mol ($H_2O_l \longrightarrow H_2O_g$)

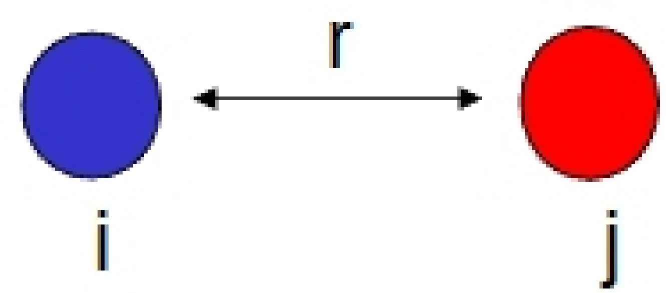
Intermolecular interactions are weaker than intramolecular interactions, but It is determining solubility, boiling points, vapor pressure, melting points…. These properties are of importance in determining the behavior of compound in chromatography and other separation methods

A useful general principle in separation is **like dissolves like**. In other words, a molecule will interaction most strongly with the phase or solvent that is most similar to it in its chemical characters.

Question: glucose (1) → Water (2)
naphthalene (2) → Hexane (1)

Intermolecular Interactions

The intermolecular interactions can either be attactive or repulsive in nature.



$$E_{total} = A/r^{12} - \Sigma B/r^{z}$$

Where: E_{total} = net total energy of interactions

A = constant describing repulsive forces between i and j

B = constant describing attractive forces between i and j

z = constant for a given type of attractive force

Lennard-Jones potential: z=6

1. Dipole-dipole interaction

2. Induction interaction

3. Dispersion interaction (London forces)

} van der Waals forces

4. Hydrogen bond

5. Lewis acid-base interactions

- **Electrostatic interaction (Coulombic) (hard interactions)**
- **Electron transfer (sharing electron) (soft interactions)**