Fundamentals of Distribution Separations (III)

(08/30/13)

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

$$C_i = \exp\left(\frac{-\Delta\mu^0}{RT}\right)$$ *solubility*

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

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

$$\Delta H_i^0 = \Delta H_{i,\beta}^0 - \Delta H_{i,\alpha}^0$$

$$\Delta H^0 = E_L + E_I + E_D + E_{AB}$$

Quantitative Approach for the Strength of Molecular Interactions (II)

A more quantitative approach in estimating the strength of molecular interactions is to use various scales that describe molecular polarity.

(a) Polarizability
(b) Dipole Moments
(c) Solubility parameters

(b) Dipole Moments

(1) The dipole moment (μ) is a measure of the electron distribution in a compounds
(2) The dipole moment of a compound is determined by
- The electronegativity of all atoms in the compound
- The way in which these atoms are connected and the 3-D structure

(3) Examples of electronegativities for some elements

Element	Electronegativity (Pauling Scale)
Hydrogen	2.1
Carbon	2.5
Sulfur	2.5
Nitrogen	3.0
Oxygen	3.5
Fluorine	4.0
Chlorine	3.0
Bromine	2.8
Iodine	2.5

(4) For a non-symmetrical molecule made up of neighboring atoms with different electronegativities, a partial separation of positive and negative charge is produced (i.e., a dipole).

(5) The magnitude of the dipole moment in a compound is given by

$$\mu = e\, d$$

Where: μ = dipole moment (Debye units)
e = Magnitude of the charge (electrostatic units)
d = Distance (cm)