ABSTRACT

Physicochemical behaviors of solutions are very essential to get idea about the intermolecular interactions in solute-solvent systems. Precise understanding of physicochemical and thermophysical behavior of solution has great importance in appropriate designing of industrial methods.

The branch of physical chemistry deals with the change in physicochemical and thermodynamic properties when two or more components are mixed homogeneously is called solution chemistry. The solubility of substances and the effect of solubility on the chemical properties of both the solute and the solvent also fall in the perview of solution chemistry. The homogeneous mixing of more than one components gives rise to solutions which does not behave ideally. The deviation from ideality is defined with many many physicochemical and thermodynamic parameters which are helpfull to investigate the different interactions in solution.

There are mainly three kinds of interactions in solution such as solute-solute, solute-solvent and solvent-solvent species in case of non-electrolitic solution and ion-ion, ion-solvent and solvent-solvent species in case of electrolitic solution. The forces prevailing in the solution may be either attractive or repulsive which depend on closer approach of like or unlike charges. The investigations on solution properties provide some valuable information understanding the variation in ionic structure, ionic mobility and thermodynamic properties of different electrolytes and non-electrolytes in their aqueous or non- aqueous solutions.

The thermodynamic parameters such as enthalpy, entropy, changes in free energy etc. can be estimated qualitatively which enable us to study the ion-solvent interactions of solute-solvent system. The information about the ion-solvent interactions can be obtained from physicochemical properties like density, viscosity, refractive index, conductance, ultrasonic speed refractive index etc. of the electrolyte solution using solvation approaches.

Bioactive compound are extra nutritional constituents which is present in very small amount in foods and has effect on living cells. The effect may be positive or negative. The positive effect means beneficial or good effect and negative effect means adverse or toxic effect. The beneficial properties of bioactive compounds are defined on the basis of pharmacological activities. Various physiological functions are carried out by bioactive compounds like phenolic compounds, mannitol, glucose, caffeine, Organosulfur compounds,

isothiocyanates, nicotinamide etc. in human body. Other compounds such as the amino acid, flavonoids, fatty acids, anthocyanins, phytosterols, glucosinolates, prebiotics, polyphenols, flavonoids, carotenoids, caffeine, carnitine, choline, coenzyme, creatine, dithiolthiones, phytoestrogens, polysaccharides, taurine etc. have favourable health effects Similarly minerals in very small quantities are present in foods in the form of salts and take key role in the formation of body substances like hormones, enzymes etc.

The intermolecular interactions at microscopic and macroscopic level can be studied from physicochemical properties like viscosities, densities, excess molar enthalpies, refractive indices, isentropic compressibility etc. which can be measured easily and very accurately in laboratory. The excess properties are also important parameters to investigate the nature and extend of solute-solvent interactions in the solution.

From the volumetric study we determined many physicochemical parameters like limiting apparent molar volume, (ϕ_V^0) and experimental slopes (S_V*) using Masson equation which provide the information about the solute–solvent and solute–solute interactions respectively. We also determined the limiting apparent molar volumes of transfer ($\Delta\phi_V^0$) which signifies the presence of various hydrophobic–hydrophilic and hydrophobic–hydrophobic interactions between the solute and co-solute in in electrolytic and non-electrolytic solutions. The limiting apparent molar expansibilities (Φ_E^0) can be calculated from ϕ_V^0 values at different temperatures which provide the idea about the structure making or breaking properties of the solutes.

The viscosity study was used to evaluate the viscosity A and B coefficients from Jones–Dole equation which signify the solute-solute and solute-solvent interactions, respectively. Molar free energy of activation of viscous flow of the solvent, $\Delta\mu_1^0$ and solute, $\Delta\mu_2^\circ$ were estimated using viscosity B and limiting apparent molar volume, (ϕ_V^0) values from the equations proposed by Feakins et al. These parameters were used to examine the stability of ground state over transition state for viscous flow. The study of viscous property of any pharmaceuticals, foodstuffs, cosmetics is compulsory for getting the idea whether its viscosity is suitable for the long term use or not and also its expiry information.

The molar refraction, R_M was calculated from the Lorentz–Lorenz relation using the refractive index, the molar mass and the density of solution. Some thermo-physical parameters like critical constants, transport properties and heat capacity may be calculated

from refractive index of any solution. The molar refraction, R_M values give idea about solute-solvent interactions in solution.

Study on of transport and acoustic properties of electrolytes provides significant information about molecular interactions in aqueous and non-aqueous solutions. Another important property is the ion solvation which has enormous applicability in different fields like chemical synthesis, determination of reaction mechanisms, extraction of compounds, non-aqueous batteries etc.

Inclusion complexes play a significant role in the drug formulation and drug delivery process in pharmaceutical industries. Some others methods used to improve the solubility of drugs molecules are solid dispersion, micronization, solvent deposition etc. All the approaches are used for improving dissolution rate, miscibility and bioavailability of sparingly soluble drugs. But each method has some boundaries and advantages. Inclusion complexation with cyclodextrin is the most efficient method to improve the solubility of weakly soluble drugs. Cyclodextrin by the formation of Inclusion complex are capable to modify the physicochemical properties of drugs such as solubility, particle size, thermal behavior and thus providing a highly water miscible amorphous forms. The CDs are not only capable of enhancing the dissolution rate but also bio-availability of the sparingly soluble drugs. The permeation of drugs through various biological membranes can also be improved by formation of drug-cyclodextrin inclusion compounds.

The formation of inclusion complex can be characterize by many and spectroscopical techniques such as NMR, FT-IR, UV-Vis spectroscopies as well as physicochemical techniques such as surface tension, conductance, refractive index, density and viscosity studies. In ^{1}H NMR, the considerable chemical shifts of H3 and H5 protons of cyclodextrins and the protons of hydrophobic part of the guest molecule may be regarded as the formation of inclusion complexes. The mechanism of formation of inclusion complex may be explained using ^{1}H NMR and 2D ROESY NMR spectroscopies. The significant shift of different groups of ICs from the host and guest molecules are observed in FT-IR spectra which is also the proof of formation inclusion complexes. The surface tension and conductance study are some reliable techniques for characterization and evaluation of stoichiometry of inclusion complex. The stoichiometries of the inclusion complexes were also estimated from Job's plot of UV-visible spectroscopy. The association/binding constants of various host-guest systems were calculated from Benesi-Hildebrand equation.