Molecular Interaction Study of Sodium Nitroprusside in AQUO Organic Solvent Media

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ABSTRACT - Density and ultrasonic velocity have been measured for sodium nitroprusside in aqueous solutions of CH_3OH and ethylene glycol. A quantitative relationship has been established among the thermodynamic properties like sound velocity (U), adiabatic compressibility (Ks), intermolecular free length (L_f), apparent molar volume ($V_Ø$), limiting apparent molar volume ($V_Ø^0$) and its constant (S_v). From the obtained values, molecular interaction study has been made successfully in the light of these acoustical properties through hydrogen bonding between solute and solvent mixture.

Keywords: Sodium nitroprusside, Ultrasonic velocity, apparent molar volume, acoustical impedance, molecular interaction, hydrogen bonding.

I. INTRODUCTION

In the recent years ultrasonic velocity measurements are helpful to interpret solute-solvent, ion- solvent, solvent-solvent interaction in aqueous and non aqueous medium[1-4].Mishra et al have investigated ultrasonic velocity and density in non aqueous solution of metal complexes and evaluate acoustic properties of metal complex[5]. The interaction helps in better understanding the types of solute and solvent i.e. whether the added solute modifies or distorts the structure of solvent. Apparent molar volume gives valuable information about ion-ion and ion-solvent interaction in solution [6-10] .The addition of organic solvent to an aqueous solvent of electrolyte brings about the change in ion salvation that result a large change in reactivity of dissolved electrolyte[11-12]. The transition metal plays a vital role in life system because of natural presence in vitamins, proteins and enzyme. Sodium nitroprusside (SNP), a Fe (II) ion complex is an effective drug which rapidly lowers blood pressure and causes vascular smooth muscle relaxation. It is also used in a urinalysis test. In the presence of buffers it is used as a reagent for ketone strips which test the ketone level in the urine of a diabetic. It is used by forensic chemists in Simons fast for the identification of illicit substances[13]. Thus an attempt has been made to elucidate the ion-ion and ion – solvent interaction of SNP in aqueous methanol and ethylene glycol through ultrasonic velocity and density measurement.

II. EXPERIMENTAL

A synthetic method of preparation of SNP has been reported[14]. The density was determined using a specific gravity bottle by relative measurement method. The ultrasonic velocity was measured by ultrasonic interferometer having frequency $2MH_Z$ (Mittal Enterprises, model no F-81).

Using the measured data the following volumetric compressibility parameters have been calculated using the standard relations,

Ultrasonic velocity (U) $=\lambda \times F$.

Adiabatic compressibility (Ks) $=1/U^2d$

Intermolecular free length $(L_f)=K_j\, Ks^{1/2}$

Relative association $(R_A)=(d/d0) \times (U0/U)^{1/3}$

The apparent molar volume (V_ϕ) has been determined employing the relation.

$$V_\phi = 1000(d_0-d)\,(cd_0)^{-1}+M_2d_0^{-1}$$

Where M_2 is the molecular weight of solute concerned

d and d_0 denote the densities of solution and solvent respectively

c is the concentration of the solution.

The limiting apparent molar volume, V_ϕ^0 are obtained from the following equations,

$$V_\phi = V_\phi^0 + S_V C^{1/2}$$

Where S_V are the slope of the linear variation.

III. RESULT AND DISCUSSION

The desired parameters such as adiabatic compressibility (Ks), inter molecular free length (L_f) , Relative association (R_A), apparent molar volume (V_φ), limiting apparent molar volume (V_φ^0) and its constant (S_V) have been studied. The density decreases with mole fraction of CH_3OH but increases with the mole fraction of ethylene glycol . The decrease in density in case of CH_3OH+ water indicates the decrease in solvent-solvent or ion-solvent interaction or structure breaking properties of sodium intraprusside. But addition of ethylene glycol to water have rigidified the three dimensional structure of water forming a strong hydrogen bond between solvent moleuculs[15-16] . It also indicates the structure forming properties of sodium nitroprusside in ethylene glycol+ water.

Ultrasonic velocity increases with increase in the concentration of sodium nitroprusside in aqueous CH_3OH but it is found to be decreased in aqueous ethylene glycol. The increase in ultrasonic velocity in these solutions may be attributed to the cohesion brought about by the hydration[17].

The adiabatic compressibility decreased with increasing in the concentration of solute in all aqueous solvent solution except n-propanol+water. The decreasing adiabatic compressibility observed for sodium intraprusside in CH_3OH +water and ethylene glycol +water confirm the calculation drawn from the velocity data. The increasing electrostrictive compression of water around the solute molecules results in a large decrease in the compressibility of solutions. The decrease in the compressibility implies that the molecular association are enhanced in these systems with increase in the solute content as the new entities (formed due to molecular association become compact and less compressable[18] .The compressibility appeared to decrease with increasing hydrogen bond strength between solute and solvent molecules. The larger decrease in compressibility of nitroprusside in DMSO +water indicates larger molecular association capacity than other solvents. But increase of adiabatic compressibility with increase in concentration of solution may be due to collection of solvent molecules around ion[19] supporting weak ion-solvent interaction. This indicates that there is significant solute solvent interaction.

The intermolecular free length (L_f) is a predominant factor in salvation chemistry. Intermolecular free length depends on the intermolecular attractive and repulsive forces. In the present investigation the intermolecular free length is found to decrease with increase in concentration of nitroprusside indicating a significant molecular association between solute and solvent molecules suggesting a structure promoting behaviors on addition of solute.

Decrease in relative association (R_A) is due to the breaking up of the solvent molecules on adding the solute whereas increase as R_A may be due to the solvation of solute[20] . In all the systems R_A increases with increase in concentration due to the increase in electrostatic attraction. From this data it can be said that ion-ion interaction overcomes the ion-solvent interaction.

The values of V_φ are positive for CH_3OH whereas positive for ethylene glycol.

Further the negative values of V_φ indicate electrostatic solvation of ions[21] .

The volume behavior of solute at infinite dilution is satisfactorily represented by V_φ^0 which independent of ion-ion interaction and provides information concerning ion-solvent interaction. The values of V_φ^0 are positive for CH_3OH shown in Fig. 1 where as these are negative for ethylene glycol (Fig. 2).Thus in ethylene glycol solutions predominance of ion-solvent interaction is again proved by negative V_φ^0 values. However in CH_3OH solutions positive values of V_φ^0 suggest that ion-ion interactions predominate.

The Sv exhibits negative values in CH_3OH systems suggesting the presence of stronger ion-ion interactions and less complex formation occurring in the systems. The values of Sv which exhibit positive in ethylene glycol reflect the existence of weak ion-ion interactions and predicting the complex formation taking place in the systems.

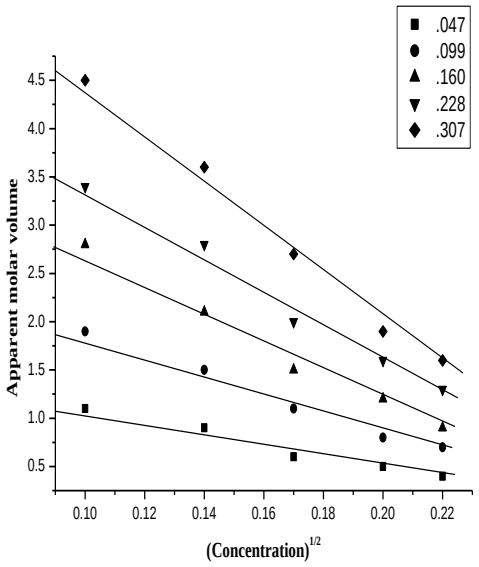

Figure 1 – Plot of apparent molar volume(V_φ) verses $C^{1/2}$ for sodium nitroprusside in different mole fraction of CH_3OH in water.

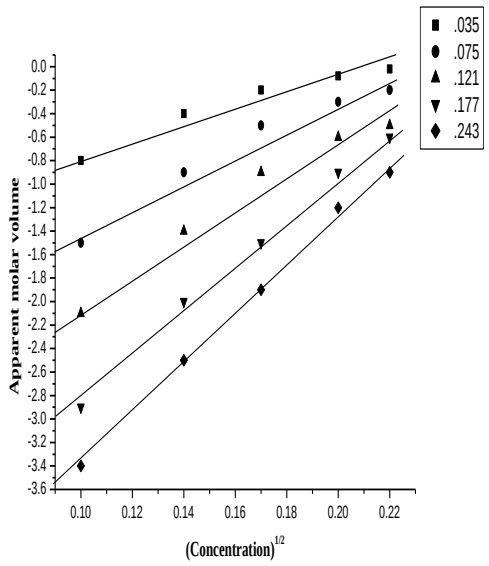

Figure 2 – Plot of apparent molar volume(V_φ) verses $C^{1/2}$ for sodium nitroprusside in different mole fraction of ethylene glycol in water.

IV. CONCLUSION

From the magnitude of ultrasonic parameters it can be concluded that the larger ion-solvent interaction will exist in ethylene glycol than methanol. Thus sodium nitroprusside is an effective structure maker in aqueous ethylene glycol.

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VI. REFERENCES

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