International Journal of Current Research and Review
DOI: http://dx.doi.org/10.31782/IJCRR.2018.5963

Research Article

IJCRR
Section: General Science
Sci. Journal Impact Factor: 5.385 (2017)
ICV: 71.54 (2015)

UV-Visible, Transport And Solvation Analysis of An Electrolyte AT 308.15K

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ABSTRACT

The present study elaborates the experimental details on the transport features and properties of peptide with electrolyte in non-aqueous solutions of different temperatures. The measured quantities are density, viscosity, ultrasonic velocity, conductivity, solvation number and thermodynamical parameters at different temperatures. The results are discussed in terms of solute-solute, solvent-solvent, solute-solvent interaction of electrolyte in non-aqueous solution. Agar well diffusion method showed appreciable antifungal activity against aspergillus Niger. An attempt is made to correlate the ultrasonic, spectroscopic and biological study of the sample at different temperatures.

Key Words: Ultrasonic velocity, Thermodynamic parameter, Solvation, Antimicrobial study

INTRODUCTION

Ultrasonic study on amino acids in non-aqueous solution of electrolytes and non-electrolytes provides useful information in understanding the behaviour of liquid systems [1-4]. Amino acids are the structural units (monomers) that make up proteins. They join together to form short polymers chain called peptides [5].

Sodium Chloride is one of the most well-known and widely used chemicals, also known as table salt. It is best known as table salt and is used widely used in the food industry for flavouring and preservation [6]. Hence it is important to analyse Density Functional theory of the title compound for upcoming studies. In addition to, researches are also very helpful for the theoretical and experimental evidences since computational methods are responsible to characterize the molecule because of their efficiency and exactness with regard to the observation of molecular properties.

Renato Tomas et al [7] reported Transference numbers of sodium chloride in formamide + water mixtures at 298.15K from potential difference measurements. Palaniswamy et.al [8] reported Growth and characterization of nonlinear optical material: Glycine Sodium Chloride. Yasmin Akhtar et.al [9] reported Molecular interaction studies of Glycylglycine in aqueous NaCl and NaBr at different temperature. Yasmin Akhtar et.al [10] reported Ultrasonic and thermodynamic study of glycyl in aqueous electrolyte solutions at 303 K. Gad Fischer et.al [11] reported The FT-IR spectra of glycine and glycylglycine zwitterions isolated in alkali matrices. Nidhi Sharma et.al [12] reported Ultrasonic study and allied physical parameters of Uni-univalent mixed electrolytes in formamide.

Literature survey reveals that, there is no ultrasonic and antimicrobial studies for title compound peptide with electrolyte in non-aqueous medium. In the present investigation, the polar protic solvent is taken along with a peptide and electrolyte, the solutions were prepared at different molalities with peptide and a fixed concentration of electrolyte. The thermodynamic parameters such as internal pressure, free volume and solvation number were computed. The results arrived from these parameters were correlated with ultrasonic and antimicrobial studies.

MATERIALS AND METHODS

Experimental Details

Ultrasonic velocity was measured using digital ultrasonic interferometer of fixed frequency 2MHz (Model F-81 Mittal enterprises, New Delhi) with an accuracy of ± 0.2 m/s. The

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ISSN: 2231-2196 (Print) **ISSN:** 0975-5241 (Online)
Received: 24.08.2018 **Revised:** 28.09.2018 **Accepted:** 15.10.2018

density of the non-aqueous peptide with electrolyte solutions were measured using Anton Paar DMA 4100 Digital densitometer with an accuracy of ± 0.0001 gm/cc. The viscosities of the solutions were measured using Cannon Fenske viscometer (±0.1 %) error with the experimental solution was immersed in a temperature controlled water bath. The time of flow was measured using a stop watch with an accuracy of 0.1 sec.

Computation

The measured data were used to calculate the thermodynamic, solvation and electrochemical parameters using the standard relations,

Internal Pressure $\prod_i = b\,RT\,(K\eta/U)^{1/2}\,\rho^{2/3}/M_{eff}^{7/6}\ (10^9)$ Pa -- 1

Free volume $V_f = [M_{eff}\,U/K\,\eta]^{3/2}\ (10^{-9})\ m^3$ ---- 2

Solvation number $n_s = n_i/n_f\,[1-\beta_{soln}/\beta_{solv}]$ ---- 3

RESULTS AND DISCUSSION

Table 1: UV spectral analysis of the samples

Samples	200-400 nm
Formamide	270.0 272.5
Glycyl-L-glycine	273.7 710.5
Sodium chloride	276.2 330.7
Glycyl-L-glycine + Sodium chloride + Formamide solution	268.7 274.9 336.9

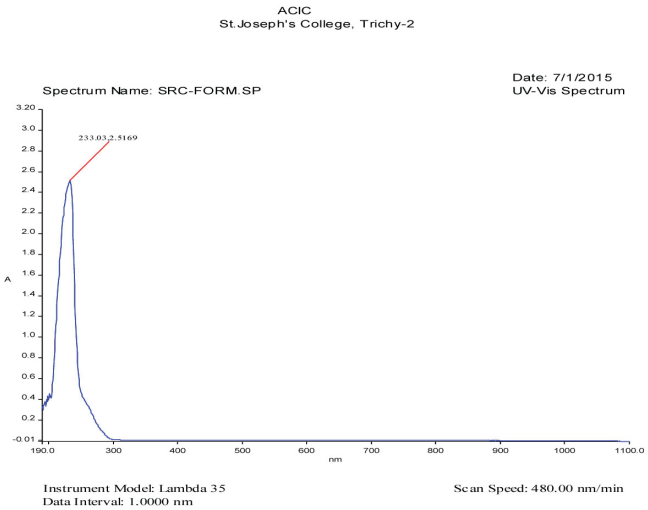

Figure 1: UV-Visible Spectrum of Formamide.

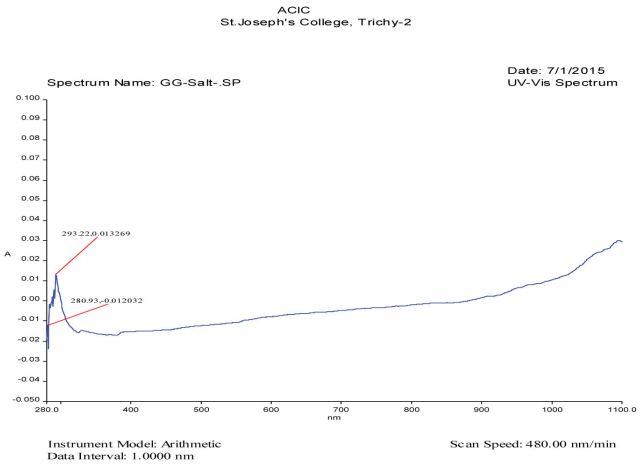

Figure 2: UV-Visible Spectrum of Glycyl-L-glycine.

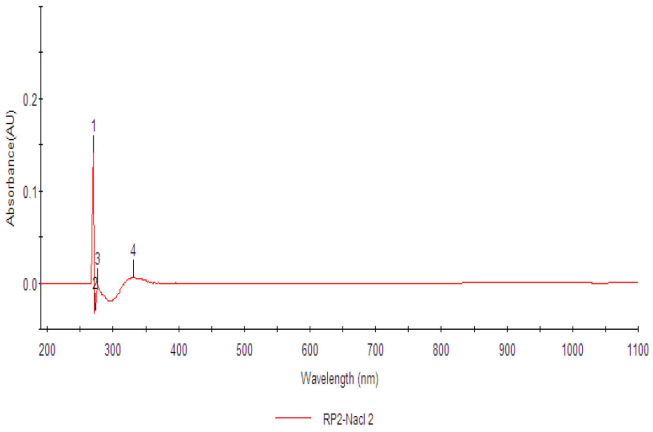

Figure 3: UV-Visible Spectrum of Sodium Chloride.

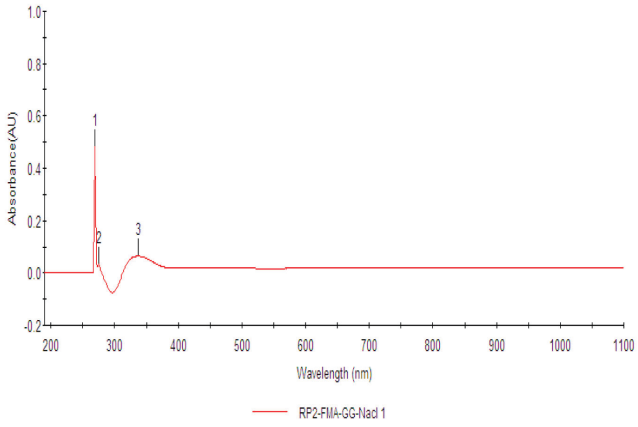

Figure 4: UV- visible spectrum of solution.

UV Spectroscopy

In the UV-Visible spectrum of formamide the peaks at 270 and 272.5 nm are assigned to π-π* transitions in the $\diagdown\!\!\diagup C{=}O$ group in formamide intensity of the peaks are 0.005 and 0.004 respectively.

In Glycyl-L-glycine the -π* peak is found at 273.7 nm with intensity of 4.0 when Nacl is considered along a sharp peak is observed at 270 nm with the intensity of 0.15.

In the mixture of Glycyl-L-glycine and NaCl, there is a intense peat at 268.7 nm of intensity 0.54 nm is found. The small peak at 275 nm of intensity of 0.03 should be due to π-π* transition in the solvent formamide. At 336.9 nm a broad peak is observed with an intensity of 0.06. this broadening is indicative of charge transfer between solutes and solvent. This peak is not found either in the spectra solute or solvent. The Glycyl-L-glycine, sodium chloride and formamide should form a cluster through H-bonding. The charge is being transferred from one molecule to another. The intermolecular charge transfer transition should be the cause of the new peak which is closer to the visible region. The cluster formation and charge transfer interaction are depicted below.

Formamide is a H-bonding solvent with high dielectric constant. It is a highly polar solvent. Nacl is a ionic molecule. In the mixture NaCl in formamide the Na^+ and Cl^- ions are well solvated. This can be observed by the increase in intensity of 270 nm peak from 0.05 to 0.15.The small peaks at 272.5 nm, 276.2 nm, 270 nm are of very low intensity (0.002). The new peak at 330.7 nm of 0.005 intensity is the charge – transfer band between $Cl^-$and formamide. Thus the ion-solvent interaction between NaCl and formamide can be represented as follows.

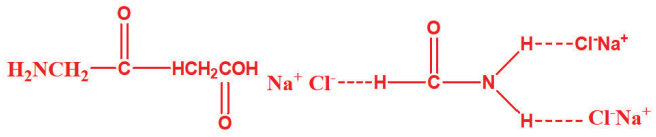

Figure 5: Interaction between the components of the solution.

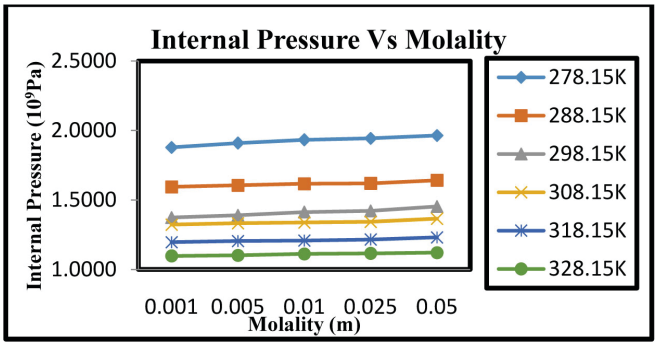

Figure 6: Internal pressure.

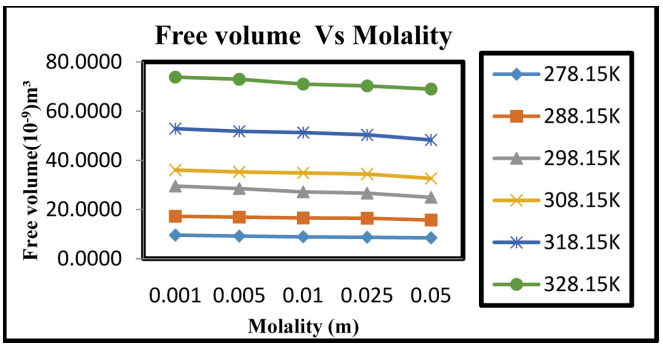

Figure 7: Free volume.

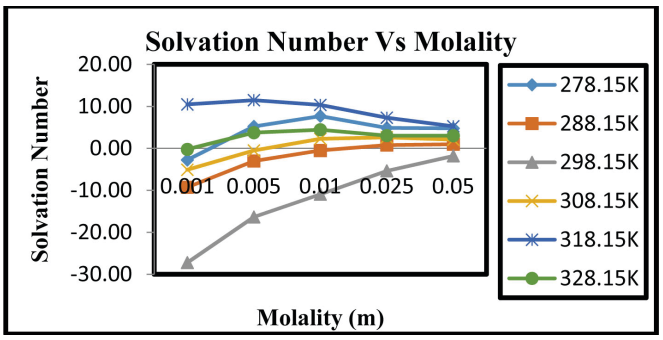

Figure 8: Solvation Number.

Ultrasonic study

Internal pressure and Free volume

Internal pressure is the resultant of the forces of attraction and forces of repulsion between the molecules of the solution. Internal pressure increases with increasing concentration at all temperatures. This increasing value indicates that there is a strong peptide-electrolyte-amide interaction prevails in the solution. Hence the presence of solutes enhances the structure of the solvent [13]. Free volume is the average volume in which the centre of a molecule can move due to the repulsion of the surrounding molecules. Free volume decreases with increase in concentration. Decrease in the free volume and the increase in the internal pressure suggest that the cohesive forces are dominating in the solution of ternary mixtures.

Solvation Number

Solvation is the attraction and association of molecules of the solvent with molecules or ions of a solute. The ternary mixture of non-aqueous solution exhibit a positive solvation number above the room temperature for almost all concentrations, but it exhibits negative solvation number below room temperature. Positive values of solvation number suggest that the compressibility of the solution at all the molalities will be less than that of the solvent. Negative values of solvation number emphasizes that the solutions are more compressible than solvent.

Salient features of the samples

Test organisms

The test microorganisms of *E.Coli* and Fungus *Aspergillusniger*, are obtained from National Chemical Laboratory (NCL) Pune. Antibacterial and antifungal properties of the ligand and its complexes were tested *in vitro* against the bacterial species *Escherichia coli* and fungal species *Aspergillusniger,*by the disc diffusion method.

Table 2: The computed values of internal pressure, free volume and solvation number of non- aqueous ternary solutions, at different concentrations are shown in the table

Molality (m)	Internal pressure (10^9) Pa					
	278.15 K	288.15 K	298.15 K	308.15 K	318.15 K	328.15 K
0.001	1.8787	1.5945	1.3740	1.3231	1.1968	1.0974
0.005	1.9098	1.6059	1.3903	1.3332	1.2048	1.1023
0.01	1.9330	1.6171	1.4132	1.3383	1.2086	1.1124
0.025	1.9437	1.6196	1.4216	1.3433	1.2155	1.1158
0.05	1.9641	1.6423	1.4530	1.3655	1.2313	1.1216
Free volume (10^{-9})m^3						
0.001	9.6015	17.2287	29.5209	36.0380	52.8519	73.8166
0.005	9.1784	16.8847	28.5243	35.2624	51.8041	72.9419
0.01	8.8768	16.5487	27,1580	34.8689	51.2998	70.9833
0.025	8.7111	16.4485	26.6395	34.4247	50.3468	70.2428
0.05	8.4615	15.7185	24.9504	32.6455	48.2902	68.9394
Solvation Number						
0.001	-2.76	-9.29	-27.22	-5.10	10.48	-0.24
0.005	5.23	-3.02	-16.34	-0.54	11.48	3.74
0.01	7.68	-0.51	-10.93	2.27	10.36	4.44
0.025	4.88	0.76	-5.36	2.61	7.31	3.03
0.05	4.76	0.97	-1.81	2.08	5.26	302

Table 3: The obtained results are tabulated as follows:

S. No	Name of micro organism	Zone of inhibition in mm				
		FMA	NACL	GG + NACL	GG	Standard
1.	E.coli (NCIM 2065)	13	16	18	10	38
2	Aspergillus niger	12	14	16	16	30

Standard –Ciprofloxacin 5 µg/disc for bacteria; Nystatin 100 units/disc for fungi.Solvent –DMSO

Figure 9: Antibacterial activity.

Figure 10: Antifungal activity.

The zone of inhibition for E.Coli in formamide 13 mm, sodium chloride is 16 mm, Glycyl-L-glycine is 10 mm and standard is 38 mm. The zone of inhibition for Aspergillus niger in formamide is 12 mm, sodium chloride is 14 mm, Glycyl-L-glycine is 16 mm and standard is 30 mm. In the recent study, the non- aqueous solution of Glycyl-L-glycine with Sodium Chloride acts as sensitive in both case such as E.Coli and Aspergillus niger (i.e) this combination may act as an disinfectant.

CONCLUSION

Ultrasonic is a versatile non-destructive technique and highly useful for investigation of various physico chemical properties such as solvation number of the solutions. UV-Visible spectroscopy results indicates that the charge transfer between solutes and solvent. Glycyl-L-glycine has also been reported to be helpful in solubilizing recombinant proteins in E. Coli. Increase in the internal pressure indicates that there is strong peptide-amide-electrolyte interaction prevails in the solution. Solvation number supports the thermodynamical behavior. It is identified that the ternary non-aqueous solution may act as sensitive in both the case E. Coli and Aspergillus niger hence, this combination may act as an disinfectant. The results obtained from spectroscopic study is being correlated with thermodynamical and biological studies.

ACKNOWLEDGEMENT

The authors are thankful to ACIC Instrumentation Centre St. Joseph College, Tiruchirappalli, for the UV-Visible study and Periyar College of Pharmaceutical Science, Tiruchirappalli, Tamil Nadu, India for the antimicrobial studies.

REFERENCES

1. Ezhil Pavai R, Renuka S, 2011 Thermodynamic properties of L-Threonine in aqueous solutions of KNO_3 at 303K, *International Journal of Research in Pure and Applied Physics,* 1(2), 6-10.
2. Sasikumar S, Meenakshi G, 2015 Evaluation of acoustical parameters of aqueous solution of sodium chloride and potassium chloride using ultrasonic waves, *International Journal of Research in Engineering Technology,* 4(2), 263-268.
3. Kanhekar S R, Pravina Pawar, Govind K Bichile, 2010 Thermodynamic properties of electrolytes in aqueous solution of glycine at different temperatures, *International Journal of Pure and Applied physics,* 48, 95-99.
4. Punitha S, Panneerselvam, Uvarani R, 2013 Thermodynamic properties of cellulose in aqueous electrolyte solutions at different temperature, *International Journal of Pharma and Bio Sciences,* 4(1), 540-548.
5. Sonali M, Watekar, Neha S, Chatale and Pankaj B. Gwande, 2016 *International Journal of Researchers in Bio Sciences, Agriculture and Technology*, 162-165.
6. John N, Sofos, 1983 Antimicrobial effects of sodium and other ions in foods – A Review.
7. Renato Tomas, Vesna Sokol, Perica Boskovic, Anika Turudic, 2013Transference numbers of sodium chloride in formamide + water mixtures at 298.15K from potential difference measurements, *International Journal of Electrochemical Science,* 8, 7669-7679.
8. Palaniswamy S, Balasundaram O N, 2009 Growth and characterization of nonlinear optical material: Glycine Sodium Chloride, *Rasayan Journal of Chemistry,* 2(1), 49-52.
9. YasAkhtar, 2016 Molecular interaction studies of Glycylglycine in aqueous NaCl and NaBr at different temperature. *Indian Journal of Chemistry,* 5(18), 287-290.
10. Yasmin Akhtar, Ibrahim S F, 2011 Ultrasonic and thermodynamic study of glycyl in aqueous electrolyte solutions at 303 K. *Arabian Journal of Chemistry,* 4, 487-490.
11. Gad Fischer, Xiaolin Cao, Nicholas Cox, Mathew Francis, 2005 The FT-IR spectra of glycine and glycylglycine zwitterions isolated in alkali matrices. *Elsevier Chemical Physics,* 313, 39-49.
12. Nidhi Sharma, Swagat Ebhad, Ultrasonic study study and allied physical parameters of Uni-univalent mixed electrolytes in formamide. *International Conference on Multidisciplinary Research & Practice,* 358-362.
13. Thirumaran S, Karthikeyan N, 2011 *International Journal of Chemical,* 3, 83-98.