RESEARCH ARTICLE

THERMOCHEMICAL, SOLVATION NUMBER AND ACOUSTICAL PARAMETERS OF A SULFA DRUG USING ULTRASONIC VELOCITY

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ARTICLE INFO

ABSTRACT

Measurement of ultrasonic velocity in non-aqueous electrolytic solution gives information about the behavior of solution such as molecular association and disassociation. The attraction and repulsion between the molecules of the components involved show considerable effect upon the physical and chemical properties of a solution such as density, viscosity and ultrasonic velocity. Benzene sulphonamide is one of the sulfa drug used in the treatment of gastrointestinal, duodenyl ulcer, neurological disorder are analyzed for the solution of the sample, in formamide. Adiabatic compressibility, solvation number, apparent molal volume and apparent molal compressibility are computed and analysed for Benzene sulphonamide in non-aqueous solution. The Structure making/breaking nature of the solute in the solvent is envisaged.

INTRODUCTION

Knowledge of the acoustic and thermodynamic properties are of great significance in studying physico-chemical behavior and the various interactions of the Solutions/liquids,Velocity of a sound wave in a medium is fundamentally related to the binding forces between the molecules. The variation of ultrasonic velocity and the related parameters constitute the wealth of information about the acoustic parameters of the system.The compressibility behavior of the solution provides very useful information related to intermolecular interactions. β ,Sn, φ_v, φ_k are computed using the fundamental quantities density, viscosity and ultrasonic velocity.

EXPERIMENTAL SECTION

Ultrasonic velocity was measured using an ultrasonic interferometer working at a frequency of 2MHz. Accuracy in the velocity measurement was $\pm$ 0.5ms^{-1}. Density was measured by 25ml specific gravity bottle. The weighing measurements were carried out by a digital balance with an accuracy $\pm$ 0.0001gm/cc. Viscosity was measured by Cannon Fenske type viscometer.

Computation

The following thermodynamic and acoustic parameters are computed using the formulae.

   i.   Apparent molal volume $\varphi_v = [1000/c_1\rho_o]\ (\rho_o-\rho) + (M_l/\rho_0)$ ml/mol
   ii. Apparent molal compressibility $\varphi_k = 1000/m\rho_o\ (\rho_o\beta-\rho\beta_o)$ $+ [\beta_oM/\rho_o](ml/mol.cm^2/dyne)$
   iii. Solvation number $(Sn) = n_1/n_2\ [1-\beta/\beta_o]$
   iv. Adiabatic compressibility $(\beta) = [1/u^2\rho]\ cm^2/dyne$
   v.   Specific acousticimpedance $Z=\rho u$ (Rayl)

RESULTS AND DISCUSSION

i. Apparent molal volume (ml/mol)

The variation of apparent molal volume is noticeable only at lower concentration but it remains constant at higher concentration. It is found that apparent molal volume is negative at lower molalities and it decreases as molality increases, at all temperatures is shown in fig(1). The decrease in apparent molal volume with an increase in molality suggests that the strong ion-ion interaction[1] taking place in the solution.The higher values of φ_v suggest that there is strong solute- solvent interaction occurring in the solution. The lower values of φ_v support the strong ion-ion interactions [2, 3].

ii. Apparent molal compressibility $x10^{-8}$ (ml/mol.cm^2/dyne)

The negative values of φ_k support that the sulfa drug are having structural influence on the solvent. The negative vales of φ_k support weak solute-solvent interactions[4].The values of φ_k are found to increase with increasing concentration and decrease with increase in temperature for both the system as shown in the fig(2).

iii. Solvation number (Sn)

The solvation number reflects the dynamic situation of the ion as its moves around in the solution[5]. The sign and magnitude of compressibility indicates the solvation effects. The Solvation approach is used to interpret ion-solvent interaction [6]. The ion-solvent interaction energy may be equal to intermolecular interaction energy [7]which results in zero values of solvation number. Negative Solvation number emphasizes that solution are more compressible than solvent. Negative Solvation number for various molalities is reported in literature[8]. The decrease in Solvation number with increasing molality is due to either not enough solvent molecules available for all the ions or preferentially ion- pairing occurred[9] as shown in the fig(3).

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Table (1) Apparent molal volume (ml/mol)

Molality(m)	5^0c	15^0c	25^0c	35^0c	45^0c	55^0c
0.001	-3445.48	-2688.14	-2336.51	-972.07	-5336.63	-3570.59
0.005	-568.75	-128.47	-296.95	226.90	-1007.78	-539.10
0.01	-223.14	13.39	-92.52	-73.53	-425.43	-341.56
0.015	-92.00	-167.17	-69.94	109.39	-270.35	-138.95
0.02	80.65	32.49	-32.43	29.92	-147.30	-101.49

Table (2) Apparent molal compressibility $x10^{-8}$ (ml/mol.cm^2/dyne)

Molality(m)	5^0c	15^0c	25^0c	35^0c	45^0c	55^0c
0.001	-28.80	-71.14	-83.91	-176.96	-294.42	-338.50
0.005	1.73	-2.80	-9.36	-25.85	-49.38	-58.32
0.01	3.02	2.82	0.97	-9.82	-20.61	-26.43
0.015	5.09	3.95	3.67	-2.07	-10.96	-15.69
0.02	6.53	5.95	4.67	-0.19	-5.76	-9.75

Table (3) Solvation number (Sn)

Molality(m)	5^0c	15^0c	25^0c	35^0c	45^0c	55^0c
0.001	102.39	353.41	425.19	936.43	1440.32	1657.49
0.005	-20.78	13.44	46.71	143.60	239.26	286.79
0.01	-21.73	-15.75	-7.22	51.56	99.73	128.17
0.015	-31.29	-25.61	-21.84	13.25	52.12	77.22
0.02	-36.24	-33.07	-26.72	1.61	27.29	47.68

Table (4) Adiabatic compressibility$x10^{-11}$ (cm^2/dynes)

Molality(m)	5^0c	15^0c	25^0c	35^0c	45^0c	55^0c
0.001	3.23	3.29	3.35	3.41	3.46	3.54
0.005	3.26	3.33	3.38	3.44	3.50	3.57
0.01	3.28	3.37	3.43	3.48	3.54	3.60
0.015	3.32	3.40	3.47	3.53	3.57	3.62
0.02	3.36	3.44	3.50	3.56	3.62	3.66

Table (5) Specific acoustic impedance ρu (Rayl)

Molality(m)	5^0c	15^0c	25^0c	35^0c	45^0c	55^0c
0.001	18.85	18.63	18.39	18.15	17.98	17.72
0.005	18.76	18.49	18.31	18.04	17.87	17.62
0.01	18.71	18.40	18.18	17.98	17.79	17.57
0.015	18.60	18.33	18.08	17.83	17.70	17.51
0.02	18.47	18.19	18.00	17.77	17.60	17.43

iv. Adiabatic compressibility$x10^{-11}$ (cm^2/dynes)

The orientation of solvent molecules around the solute is determined by adiabatic compressibility [10].The adiabatic compressibility is a measure of intermolecular association or dissociation or repulsion [11]. The adiabatic compressibility increases with the molality changes and rise in temperature [12]as shown in fig (4). When the salt is added to the solvent, the compressibility is lowered. This lowering is attributed to the influence of the electrostatic field of the ions on the surrounding solvent molecules, such a decrease may be due to (i) an increase in the number of incompressible molecule[13,14,15].
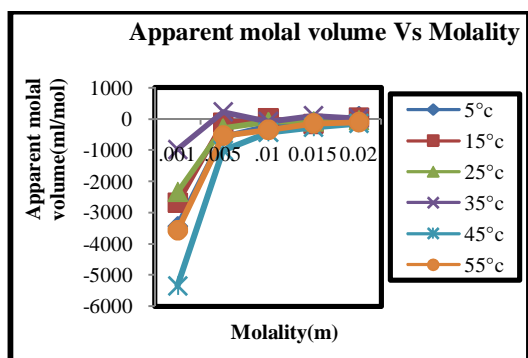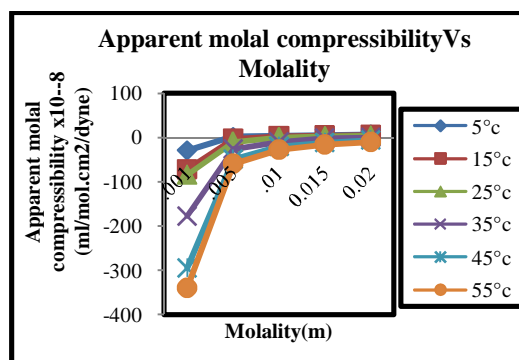

Figure (2) φ_k for Benzene sulphonamide

(ii) Structural changes occurring in the solution .This may be due to the association taking place between the molecules. When the temperature increases, the associated groups of molecules breakdown increasingly and the forces of attraction between the molecules decrease. This leads to an increase in the adiabatic compressibility of the system [16]. In the present work, the adiabatic compressibility is found to increase with increasing temperature and concentration for benzene sulphonamide.This indicates the pre-dominance of association of molecules occurring in the solution. The β increase with increasing concentration happens due to the collection of solvent molecules around ions supporting weak ion- solvent interactions [17].
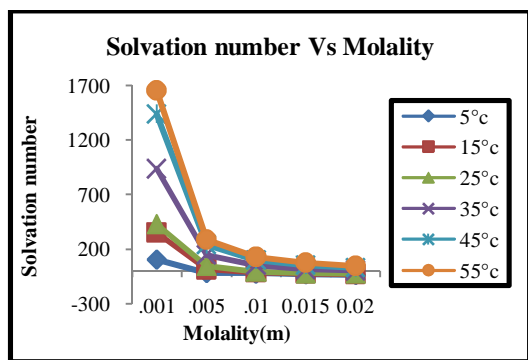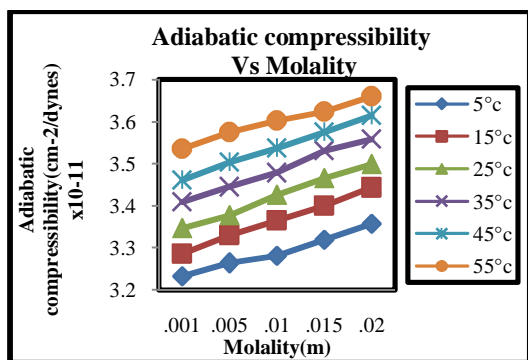

Figure (1) φ_v for Benzene sulphonamide

Figure (3) Sn for Benzene sulphonamide.

Figure(4) β for Benzene sulphonamide

v. *Specific acoustic impedance ρu (Rayl)*

The specific acoustic impedance 'Z' decrease with increasing temperature and decreasing with increase in solute concentration is shown in (fig5). This usual behavior of specific acoustic impedance emphasizes the strong solute-solvent interactions in the solutions[18,19]. Acoustic Impedance in solutions can be used as a tool to estimate the strength of intermolecular attraction [20].
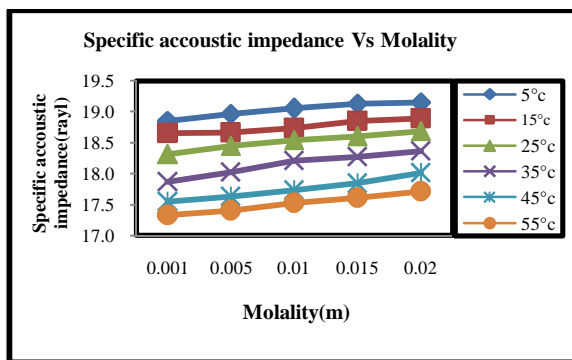

Figure (5) (ρu)forBenzenesulphonamide

CONCLUSION

A detailed analysis of thermochemical properties, φ_v, φ_k, have been carried out in the present investigation. Intermolecular interaction that is solute-solvent interaction is discussed, based on the values of Solvation number. The study of apparent molal volume and apparent molal compressibility has been proven to be useful in explaining the molecular interactions existing in solution. Both acoustical and thermochemical analysis reveals that the addition of Benzene sulphonamide in formamide enhances the structure of the solution.

Reference

1. Sathyavathi A.V. Acoustica, 28 (1973) 17.
2. Balachandran, Nature, 191 (1961) 164
3. Dhanalakshmi A.et.al., J. Acous.Soc Ind Vol 23, 1-4 (2000) 385-388.
4. Patil K.J and Ali S.T Indian Joural of Chem, Vol 22A (1983) 410.
5. Padmavathy.R,JasmineVasanthaRani.E,Seethalakshmi. K,Journal of Acoustic society of India. Vol 38, No 3, 2011 (140-143).
6. Padova.J, Isr A. Energy Comm.., (1963) 1A-823 (16pp), A-830 (23pp).
7. Modern Electrochemistry, JohnO.M, Bockris and Amulya K.N Reedy,A.plenum/rosetta Edition Vol 1 (1977).
8. Rajkotia, et.al. J .Pure and Appl .Ultrasonic's, 21 (1999) 132-135.
9. Kuppuswami.J.,Lakshmanan.A.S.,et.al.,Bull.chem.soc.J apan, 38, (1965)1610.
10. Suryanarayana C.V. J. Acou.Soc. India 7(1979) 131-136
11. Jasmine Vasantha Rani E., Seethalakshmi K.,Padmavathy.R,. And Radha.N, N.IJ. Of Pure and Applied Physics. Volume 9, Number 1 (2013), pp. 1-12
12. Syal V.K.etal., J.Acous.soc.Ind, 30(2002).
13. Shahina Islam, Waris B.N., Thermochemical acta, 424(2004)165-174.
14. Singhal S.P., Ind J. Pure and Appl.phys, vol.3 (1965)238-242.
15. Jahagirdhar D.V., Arbad B.K., Walveier A.A., Lande M..K and shankarwar A.G ., Ind J .Pure and Appl.Ultrasonics,21(1999) 108-112.
16. Bhullerk, Bhavaneet k., et.al Acoustica 73(1991) . 291-293.
17. Sonar A.N and Pawar N.S., Rasayan. J.ChemVol 3 No 1 (2010) 38-43.
18. Dhanalakshmi A., Sekar S, J. Acous .Soc. Ind, Vol-XXIV, V (1996) 14.1-14.3.
19. Geetha K., et.al. J.Acous.Soc.Ind.,Vol-30.(2002)26-28.
20. Jacobson B., J.Chem.Phys 20 (1952) 927.[20]

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