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Acoustical Study of Chalcone in Dioxane: Water Mixture in Different Concentrations

U. A. Pathare
Research Student, Department of Chemistry, R.D.I.K. & N.K.D. College, Badnera (RLy), Amravati, Maharashtra, India
S. D. Thakur
Professor, Department of Chemistry, R.D.I.K. & N.K.D. College, Badnera (RLy), Amravati, Maharashtra, India

Abstract:
Ultrasonic velocity and density measurement of chalcone - 3-bromo-2-hydroxy-5- methyl-4-chloro chalcone (3B2H5M4C1C) in dioxane-water mixture have been carried out in the concentration range $1x10^{-2}$ - $5x10^{-2}$ mole dm^{-3} and in different percentages of dioxane-water mixtures. The experimental data have been used to calculate various acoustical parameters such as adiabatic compressibility (β_s), apparent molal volume (ϕ_v), apparent molal compressibility($\phi_{k(s)}$), intermolecular free length (L_f), specific acoustic impedence (Z_s) and relative association (R_A). The results have been interpreted in terms of solute-solvent and solute-solute interactions.

1. Introduction

The study of molecular interactions on liquids provides valuable information regarding internal structure, molecular association, complex formation, internal pressure etc. Various techniques are there to study them such as NMR, microwave, ultraviolet, and infrared spectroscopy, neutron and X-ray scattering and ultrasonic investigation. Ultrasonic investigation has been the subject of exhaistive research and it finds extensive application in characterizing physico-chemical behaviour and solute-solvent interactions[1]. Recently[2], apparent molal volume, adabatic compressibility, intermolecular free length, specific acoustic impedance and relative assocation of substituted azoles in N,N-dimethyl formaldehyde in different concentrations and at different temperatures have been investigated. The present attempt is made to determine the densities and ultrasonic velocities of above ligand in 70% dioxane-water mixtures at fixed concentrations of solute (1x 10^{-2} M) for predicting the solution properties.

2. Experimental

All the chemical used were of A.R. grade. The solvents were purified by standard procedures. The solute was synthesized by standard methods. Density measurements were made by bicapillary pyknometer. The accuracy in density measurement was found to be ±0.001 g/ml. The velocity of ultrasonic wave was determined by variable path single crystal interferometer (Mittal Enterprise, Model Mx-3) of 1 MHz with accuracy of ±0.03%. The temperature was maintained at 305K with an accuracy of 0.1.The apparent molal volume (ϕ_v) and apparent molal adiabatic compressibility ($\phi_{k(s)}$) have been determined respectively from density (ds) and adiabatic compressibility (β_s) of solution by using eqs. (1) and (2) respectively.

$$\phi v = \frac{M}{ds} + \frac{[do - ds] \text{ x } 10\ 3}{m.do.ds}$$

where d_o and d_s represent densities of solvent and solution respectively, m is the molality of solution and M is molecular weight of solute.

$$\emptyset k(s) = \frac{[\beta sdo - \beta ods] \times 103}{m.do.ds} + \frac{\beta sM}{ds}$$

where βo and βs are adiabatic compressibilities of solvent and solution respectively and are calculated by,

$$\beta s = \frac{1}{U2o.do}, \beta s = \frac{1}{U2s.ds}$$

where Uo and Us are ultrasonic velocities of solvent and solution respectively. The ultrasonic velocity (U) is given by U = λ x Frequency, where λ is wave length of ultrasonic wave.

Specific acoustic impedance (Z_s), relative association (R_A) and intermolecular free length (L_f) are the functions of ultrasonic velocity are given by[3] :

Lf = K x $\sqrt{\beta_s}$, where K is Jacobson's constant.

3. Results and Discussion

In the present investigation different acoustic parameters such as adiabatic compressibility (βs), apparent molal volume (ϕ_v), apparent molal compressibility ($\phi_{k(s)}$) and acoustic impedance (Z_s), relative association (R_A) and intermolecular free length (L_f) of the solutions in different dioxane-water mixture and at different concentrations of solute are determined at 305 K and presented in Table 1.

It is observed from the table that the values of β_s decrease with decrease in percentage of dioxane in different percentages of dioxane-water mixture at fixed concentrations of solute (1 x 10^{-2} M) and with increase in concentrations in 70% dioxane-water mixture. The decrease of β_s with increase in concentration of solute may be due to aggregation of solvent molecules around the ions, supporting strong ion-solvent interactions[4].

Dioxane (%)	**Ultrasonic velocity Us (m/sec) x 10^3**	**Density d_s (g.m^{-3}) x10^6**	**Adiabatic compressibility β_s (bar^{-1})x10^{-10}**	**Intermolecular free length L_f(A^o)x10^2**	**Apparent molal volume ϕ_v(m^3/mole)x 10^{-6}**	**Apparent molal compressibility $\phi_{k(s)}$ (m^{3}mol^{-1}bar^{-1})x10^{-10}**	**Relative association (R_A)**	**Specific acoustic impedance Z_s (kg m^{-2}s^{-1})x10^6**
100	1.2040	1.0230	6.7432	49.4197	272.95	2.14	0.03388	1.2316
90	1.2360	1.0240	6.3923	48.1198	629.51	1.2	0.03329	1.2656
80	1.2401	1.0242	6.3499	47.9599	1134.24	12.44	0.03310	1.2701
75	1.2480	1.0248	6.2651	47.6386	1327.30	33.1237	0.04249	1.2789
70	1.2600	1.0252	6.1439	47.1756	1453.60	34.114	0.04217	1.2917
60	1.2801	1.0260	5.9523	46.4341	1977.11	37.2129	0.04155	1.3133

Table 1: Acoustic Parameters of (3B2H5M4CIC) in different percentage of dioxane-water mixture

Concentration of ligand(m) (mole/dm^3)	**Ultrasonic Velocity Us (m/sec) x 10^3**	**Density d_s (g.m^{-3}) x 10^6**	**Adiabatic compressibility β_s (bar^{-1}) x 10^{-10}**	**Intermolecular free length L_f(A_o) x 10^2**	**Apparent molal volume ϕ_v (m^3 mol^{-1} bar^{-1}) x 10^{-6}**	**Apparent molal compressibility $\phi_{k(s)}$ (m^{3}mol^{-1}bar^{-1}) x 10^{-10}**	**Relative association (R_A)**	**Specific acoustic impedance Z_s (kgm^{-2}s^{-1}) x 10^6**
1 x 10^{-2}	1.4601	1.0347	4.5336	40.5177	204.52	7.7588	0.03673	1.5109
2 x 10^{-2}	1.48017	1.0355	4.4087	39.9623	200.13	4.6636	0.03626	1.5327
3 x 10^{-2}	1.48018	1.0372	4.4014	39.9292	176.05	2.2073	0.03633	1.5419
4 x 10^{-2}	1.4842	1.0389	4.3107	39.7897	161.79	1.6460	0.03628	1.5419
5 x 10^{-2}	1.4881	1.0393	4.3454	39.6743	176.60	1.2883	0.03620	1.5466

Table 2: Acoustic Parameters of (3B2H5M4C1C) in different concentrations of solutein 70% dioxane-water mixture

The positive values of ($\phi_{k(s)}$) at all composition may be due to gain of compressibility of solute due to weak electrostrictive solvation of ions. The values of ($\phi_{k(s)}$) increase with decrease in concentrations of solute indicating decrease in solute-solvent interactions and increase in electrostrictive solvation of ions. The positive values of ϕ_v at all compositions and percentage of dioxane are showing that the interactions are insensitive to solvent. It is seen that intermolecular free length (L_f) increases with increase in percentage of dioxane indicating weak interaction between ion and solvent molecules. This also implies increase in number of free ions showing ionic dissociation but weak ion-ion interactions. The specific acoustic impedance (Z_s) values decreases with increase in percentage of dioxane. It also supports weak ion-solvent interaction and electrostictive solvation of ion, also the acoustic impedance increases with increase in concentration of solute.

The R_A values decreases with decrease in percentage of dioxane.

The values of ϕ_v, L_f decreases with increase in concentrations of solute. This may be due to decreasing intermolecular interactions with addition of solute forming aggregate of solvent.

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5. References

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