

## Ultrasonic Behaviour And Study Of Molecular Interactions Of Chalcone In Dioxane At Different Concentrations And In Different Percentages Of Dioxane- Water Mixture

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**Abstract:** Ultrasonic velocity and density measurement of chalcone 3-bromo-2-hydroxy-5- methyl-furyl chalcone(3Br2H5MeFuC) in dioxane-water mixture have been carried out in the concentration range  $1 \times 10^{-2}$  -  $5 \times 10^{-2}$  mole  $\text{dm}^{-3}$  and in different percentages of dioxane-water mixtures. The experimental data have been used to calculate various acoustical parameters such as adiabatic compressibility ( $\beta_s$ ), apparent molal volume( $\phi_v$ ), apparent molal compressibility( $\phi_{k(s)}$ ), intermolecular free length ( $L_f$ ), specific acoustic impedance ( $Z_s$ ) and relative association ( $R_A$ ). The results have been interpreted in terms of solute-solvent and solute-solute interactions.

### I. Introduction:

The study of molecular interactions on liquids provide 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 exhaustive research and it finds extensive application in characterizing physico-chemical behaviour and solute-solvent interactions<sup>1</sup>. Recently<sup>2</sup>, apparent molal volume, adiabatic compressibility, intermolecular free length, specific acoustic impedance and relative association of substituted azoles in N,N-dimethylformaldehyde 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 ( $1 \times 10^{-2}$  M) for predicting the solution properties.

### II. 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 pycnometer. The accuracy in density measurement was found to be  $\pm 0.001$  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  $\pm 0.03\%$ . The temperature was maintained at 305K with an accuracy of 0.1. The apparent molal volume ( $\phi_v$ ) and apparent molal adiabatic compressibility ( $\phi_{k(s)}$ ) have been determined respectively from density ( $d_s$ ) and adiabatic compressibility ( $\beta_s$ ) of solution by using eqs. (1) and (2) respectively.

$$\phi_v = \frac{M}{d_s} + \frac{[d_0 - d_s] \times 10^3}{m \cdot d_0 \cdot d_s}$$

where  $d_0$  and  $d_s$  represent densities of solvent and solution respectively,  $m$  is the molality of solution and  $M$  is molecular weight of solute.

$$\phi_{k(s)} = \frac{[\beta_s d_0 - \beta_0 d_s] \times 10^3}{m \cdot d_0 \cdot d_s} + \frac{\beta_s M}{d_s}$$

where  $\beta_0$  and  $\beta_s$  are adiabatic compressibilities of solvent and solution respectively and are calculated by,

$$\beta_s = \frac{1}{U_0^2 \cdot d_0}, \beta_0 = \frac{1}{U_s^2 \cdot d_s}$$

where  $U_0$  and  $U_s$  are ultrasonic velocities of solvent and solution respectively. The ultrasonic velocity ( $U$ ) is given by  $U = \lambda \times \text{Frequency}$ , where  $\lambda$  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<sup>3</sup> :

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

### III. Results and Discussion:

In the present investigation different acoustic parameters such as adiabatic compressibility ( $\beta_s$ ), apparent molal volume ( $\phi_v$ ), 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  $\beta_s$  decrease with decrease in percentage of dioxane in different percentages of dioxane-water mixture at fixed concentrations of solute ( $1 \times 10^{-2} M$ ) and with increase in concentrations in 70% dioxane-water mixture. The decrease of  $\beta_s$  with increase in concentration of solute may be due to aggregation of solvent molecules around the ions, supporting strong ion-solvent interactions<sup>4</sup>.

**Table 1**

(a) Acoustic Parameters of (3Br2H5MeFuC) in different percentage of dioxane-water mixture

Dioxane (%)	Ultrasonic velocity $U_s$ (m/sec) $\times 10^3$	Density $d_s$ ( $g \cdot m^{-3}$ ) $\times 10^6$	Adiabatic compressibility $\beta_s$ ( $bar^{-1}$ ) $\times 10^{-10}$	Intermolecular free length $L_f(A^\circ) \times 10^2$	Apparent molal volume $\phi_v$ ( $m^3/mole$ ) $\times 10^{-6}$	Apparent molal compressibility $\phi_{k(s)}$ ( $m^3 mol^{-1} bar^{-1}$ ) $\times 10^{-10}$	Relative association ( $R_A$ )	Specific acoustic impedance $Z_s$ ( $kg \cdot m^{-2} s^{-1}$ ) $\times 10^6$
100	1.3481	1.0246	5.3711	44.1089	111.86	-11.2926	0.9697	1.3812
90	1.4201	1.0297	4.8162	41.7683	86.38	-16.3000	0.9638	1.4622
80	1.4401	1.4401	4.6680	41.1207	53.87	-19.8200	0.9595	1.4877
75	1.6201	1.6201	3.6282	36.5215	40.95	-1.0190	1.0056	1.6764
70	1.6600	1.6600	3.5042	35.6270	26.03	-32.5930	0.9986	1.7190
60	1.7001	1.7001	3.3335	34.7490	4.348	-6.0962	0.9933	1.7647

(b) Acoustic Parameters of ((3Br2H5MeFuC) in different concentrations of solute in 70% dioxane-water mixture.

Concentration of ligand (m) ( $mol/dm^3$ )	Ultrasonic Velocity $U_s$ (m/sec) $\times 10^3$	Density $d_s$ ( $g \cdot m^{-3}$ ) $\times 10^6$	Adiabatic compressibility $\beta_s$ ( $bar^{-1}$ ) $\times 10^{-10}$	Intermolecular free length $L_f(A^\circ) \times 10^2$	Apparent molal volume $\phi_v$ ( $m^3 mol^{-1} bar^{-1}$ ) $\times 10^{-6}$	Apparent molal compressibility $\phi_{k(s)}$ ( $m^3 mol^{-1} bar^{-1}$ ) $\times 10^{-10}$	Relative association ( $R_A$ )	Specific acoustic impedance $Z_s$ ( $kg \cdot m^{-2} s^{-1}$ ) $\times 10^6$
$1 \times 10^{-2}$	1.4921	1.0347	4.3412	39.6552	171.876	5.8836	1.0259	1.5439
$2 \times 10^{-2}$	1.5000	1.0364	4.2882	39.4124	135.207	2.7067	1.0259	1.5546
$3 \times 10^{-2}$	1.5001	1.0380	4.2814	39.3811	123.304	1.7956	1.0274	1.5572
$4 \times 10^{-2}$	1.5041	1.0405	4.2484	39.2290	96.786	1.2688	1.0289	1.5657
$5 \times 10^{-2}$	1.5081	1.0429	4.2164	39.0810	83.910	0.9555	1.0298	1.5727

The negative values of ( $\phi_{k(s)}$ ) at different percentage of dioxane water mixture, can be postulating that polar-OH group interacts with surrounding organic solvent-water mixtures through dipole-dipole interaction in such a way that the surrounding water loses its own compressibility to certain extent. The values of ( $\phi_{k(s)}$ ) increases with decreases in concentrations of solute indicating decrease in solute-solvent interactions and increase in electrostrictive solvation of ions. The positive values of  $\phi_v$  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 electrostrictive 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  $\phi_v$ ,  $L_f$  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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