Asian J. of Adv. Basic Sci.: 3(1), 2014, 200-205
ISSN (Online): 2347 - 4114
www.ajabs.org

Acoustical and Thermodynamic Properties of 4'-Fluorochalcone in Methanol and Benzene Mixtures

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(Received 01 Jan, 2015; Accepted 07 Jan, 2015; Published 16 Jan, 2015)

ABSTRACT: 4'-Fluorochalcones was synthesized and its characterization was done by Melting Point, Thin Layer Chromatography, Infra Red spectroscopy, H^1 NMR, and Mass Spectra. The ultrasonic velocities, densities and viscosities in various compositions of methanol and benzene from 0-100% (by wt.) have been measured at 303K. The experimental data was used for the determination of various thermodynamic parameters such as specific acoustical impedance(Z), intermolecular free path length (L_f), adiabatic compressibility (β), relaxation time (τ), absorption coefficient, Solvation number (Sn), absorption coefficient values $\left(\frac{\alpha}{f^2}\right)$, and Gibb's free energy (ΔG) and The results showed that the presence of molecular interaction in the present system and obtained results were interpreted in terms of solute-solute and solute-solvent interactions in these solutions.

Keywords: 4'-Fluorochalcone; Ultrasonic velocity; Thermodynamic properties; Acoustical impedance; Intermolecular free path length.

INTRODUCTION

Various chalcones were synthesized by many researchers[1-7] they are known to exhibit various biological properties viz. antimalarial, antifungal, antibacterial anti-inflammatory, antituberculosis activity. It is well known that the introduction of fluorine atom into a molecule may lead to significant effects on the biological and physical properties of compounds like; increasing membrane permeability, changes in hydrophobic bonding .the chemistry of fluorinated heterocyclic compounds has been continuously developing due to the characteristic property of fluorine atom having small atomic radius , low polarity of C-F bond, high electronegativity these properties enhances the significance biological activity of fluorinated compound like 4'- fluorochalcone so to understand the effect of addition of this compound to the solvent mixtures and to study the interaction parameters are of great importance.

The knowledge of the thermodynamic and acoustical properties of liquid mixtures with chalcones is of immense importance for understanding the molecular interactions between the components.

Acoustical properties of some synthesized chalcones of furaldehyde in different solvents have been studied by Anchal kulshrestha[8] Measurement of ultrasonic velocity and theoretical evaluation in binary liquid mixtures of alcohol and benzene has been studied by N. Santhi.[9]

In the present investigations the acoustical properties of 4'-fluorochalcone in methanol and benzene mixtures were studied. The results were interpreted in terms of molecular interactions.

MATERIAL AND METHODS

All chemicals used were of Analytical Reagent (AR) grade supplied by Rankem (USA). Binary liquid mixtures of methanol and benzene (0-100% by weight) were prepared in airtight Stoppard volumetric flasks to minimize leakage of volatile liquids. The weighing was done by using electronic balance with a precision ±0.001mg. The double walled bicapillary pycnometer was used for the measurement of

densities of mixtures with an accuracy 0.1Kg/m^3. Cannon-Ubbelohde viscometer was used for the measurement of viscosity with an accuracy of 0.05%. The flow time of solutions (ts) were measured with a digital stop clock with an accuracy of ±0.01s (Model RACER)

Abbe's Refractometer having accuracy with (±0.01 units) was used for the measurement of refractive index. The temperature of prism box was maintained constant by circulating water from thermostat at 303K.

The ultrasonic velocity of pure solvent and solutions were measured by using ultrasonic Interferometer (Mittal Enterprises) with an accuracy ±0.1 cm/s. The temperature was maintained at 303K using a precision thermostat with an accuracy of ±0.05K

Synthesis: A mixture of 4-fluoroacetophenone (1mmol) and Benzaldehyde (1mmol) was stirred for 24 hours in presence of NaOH as a catalyst the product was isolated and recrystallized from ethanol. The purity of compound was checked by Thin Layer chromatography, Melting point, and the characterization of synthesized compound was done by IR and H^{1}NMR and GCMS.

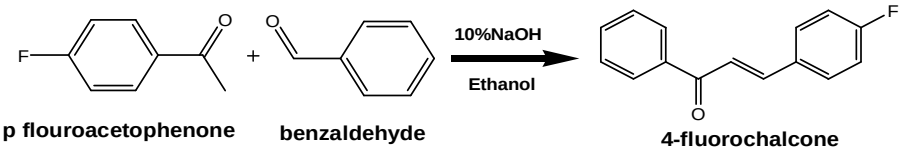


Figure 1: Structure of synthesized compound along with its IUPAC Name

Formulae: Various parameters such as adiabatic compressibility (β) free path length (Lf) and acoustical impedance (Z)[13] were calculated from the measured data using the following standard expressions:

$$\textit{Adiabatic compressibility } (\beta) = \frac{1}{U^2 \times \rho}$$

$$\textit{Intermolecular Free path length} (L_f) = K_j \times \beta^{1/2}$$

Where Kj = Jacobson's constant= 6.0816x10^4

$$\textit{Acoustical Impedance } (Z) = U \times \rho$$

By using the density, viscosity, and sound velocity some thermodynamic parameters were determined by following relations:

Effective molecular mass(M_{eff}), $M_{eff} = \sum XiMi$

Where, Xi= Mole fraction and Mi = molecular weight of ith component.

The Molar compressibility or *Wada's constant*[14] can be calculated by equation:

$$W = \frac{M}{\rho} \times \beta^{-\frac{1}{7}}$$

Where, M = relative molar mass and β = compressibility factor.

The Absorption coefficient[15] was calculated by equation;

$$\left(\frac{\alpha}{f^2}\right) = \left(\frac{8\alpha\pi^2\eta}{3\rho U^2}\right)$$

Where, η = is the viscosity of the mixture, ρ= density of the mixture

The viscous relaxation time (τ) was calculated by equation:

$$\tau = \frac{4\eta}{3\rho U^2}$$

The Solvation number (Sn) can be calculated by equation:

$$Sn = M/Mo\left\{1 - \left(\frac{\beta}{\beta o}\right)\left(\frac{100-x}{x}\right)\right\}$$

Where M and Mo are the molecular weights of solvent and solute respectively β and βo are adiabatic compressibility of solvent and solution respectively and x is number of grams of compound in 100 gm. of solution.

The Gibb's free energy can be calculated by the equation: $\Delta G = KTlog\left[\frac{KT\tau}{h}\right]$

Where, K is Boltzmann constant =1.23X10^{-23}J/K, h is Planks constant =6.626X10^{-26}Js, τ is relaxation time = 4/3ηβ

RESULTS AND DISCUSSION

The determined values of density, viscosity and ultrasonic velocity were listed in Table 1.

Table 1: Density, Viscosity, Refractive index, Ultrasonic velocity and Acoustical parameters of 4'-fluorochalcone in methanol + benzene mixtures

Wt. % of methanol	Density (ρ) g cm^{-3}	Viscosity (η) c.p	Refractive Index (n)	Ultrasonic Velocity (U) ms^{-1}	Acoustical impedance (Z) Kg.m^{-2}s^{-1}	Adiabatic compressibility (β) × 10^{-7} Kg^{-1}ms^{-2}	Free path length (Lf)×10^{-9} m
0	0.8690	0.6470	1.4915	1303.60	1132.8	6.772	50.045
10	0.8601	1.0828	1.4645	1250.66	1152.2	6.478	48.948
20	0.8529	1.1104	1.4510	1234.66	1052.1	7.691	53.335
30	0.8465	1.1059	1.4360	1217.77	1030.8	7.966	54.280
40	0.8408	1.1055	1.4240	1198.12	1007.4	8.285	55.356
50	0.8331	1.1009	1.4085	1188.88	990.48	8.492	56.043
60	0.8263	1.1025	1.3960	1184.00	978.37	8.633	56.500
70	0.8195	1.0820	1.3820	1163.35	953.42	9.016	57.746
80	0.8131	1.0689	1.3695	1154.22	945.95	9.231	58.432
90	0.8056	1.0312	1.3550	1137.77	916.59	9.589	59.553
100	0.7889	0.9791	1.3270	1111.55	876.92	10.26	61.600

The density and ultrasonic velocity values decreases with increase in the weight percent of methanol, suggests, the decrease is due to some dispersive forces due to powerful molecular dispersions.

The observed decreasing trend in ultrasonic velocity with mole fraction of methanol by addition of benzene such variations is supported by S.Thirumaran[10] increase in adiabatic compressibility (β) with increase in percentage wt. of methanol due to dispersion of solvent molecules around the solute molecules this increase is shown in Figure 2. The decrease in ultrasonic velocity and increases in β and L_f with increase in percentage of methanol values suggests predominance of solute-solvent interactions such increase suggests the hydrogen bonded association of alcohols breaks up gradually with addition of benzene is shown in Figure 3.

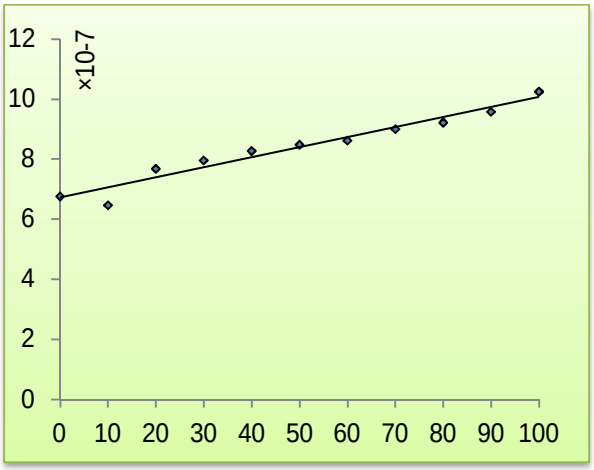


Figure 2: Relation between adiabatic compressibility and % composition of methanol

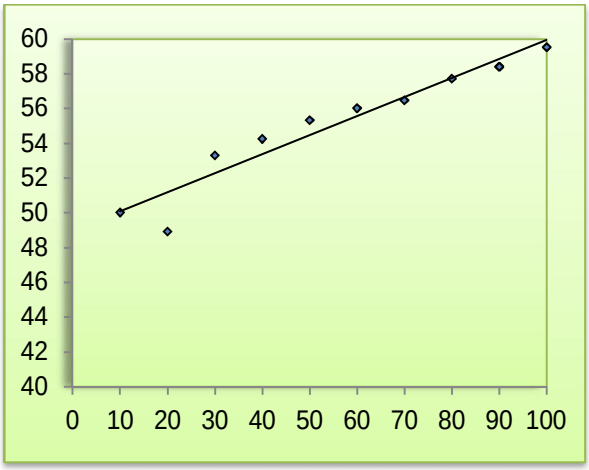


Figure 3: Relation between Free path Length and % composition of methanol

The value of relaxation time (τ) showed linear increase with increase in mole fraction indicates some specific interactions among the component at high percentage of methanol.
The degree of interaction was calculated in terms of solvation number (Sn) using N.Shakya[11] equation the decrease in the Sn with weight percent of methanol suggests the presence of solute–solute interactions the positive values suggests the structure forming tendency in methanol and benzene is shown in Figure 4.
The increase in absorption coefficient values $\left(\frac{\alpha}{f^2}\right)$ with increase in weight percent of methanol indicates the molecular interaction increases with increase in methanol.
The Gibb's free energy is found to decrease with weight percentage of methanol i.e. it shows negative deviation shown in Figure 5 which suggests the dispersion forces are present with the system, R. Pilani[12].
All these Thermodynamic parameters of 4'-Fluorochalcone in methanol + benzene mixtures represented in Table 2.

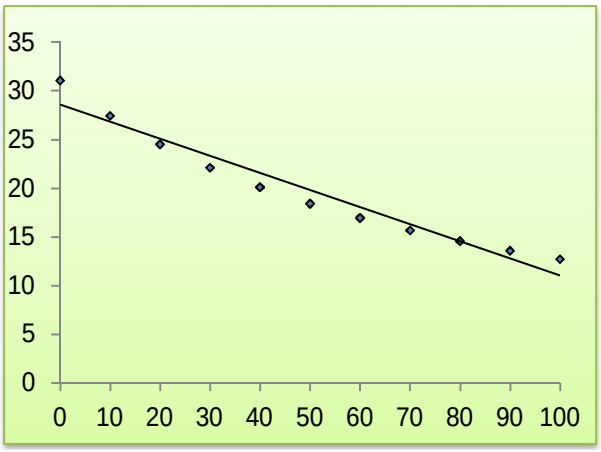


Figure 4: Relation between Solvation number and % composition of methanol

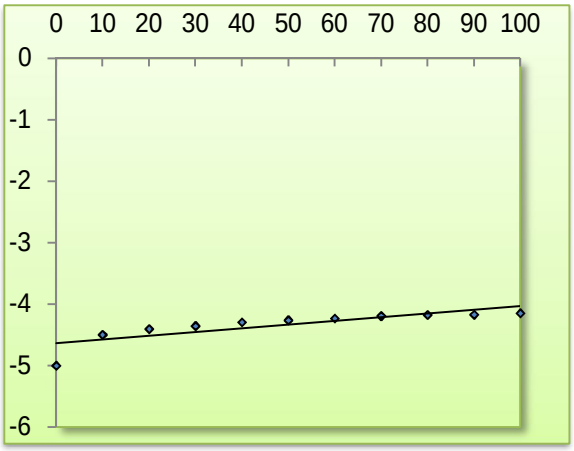


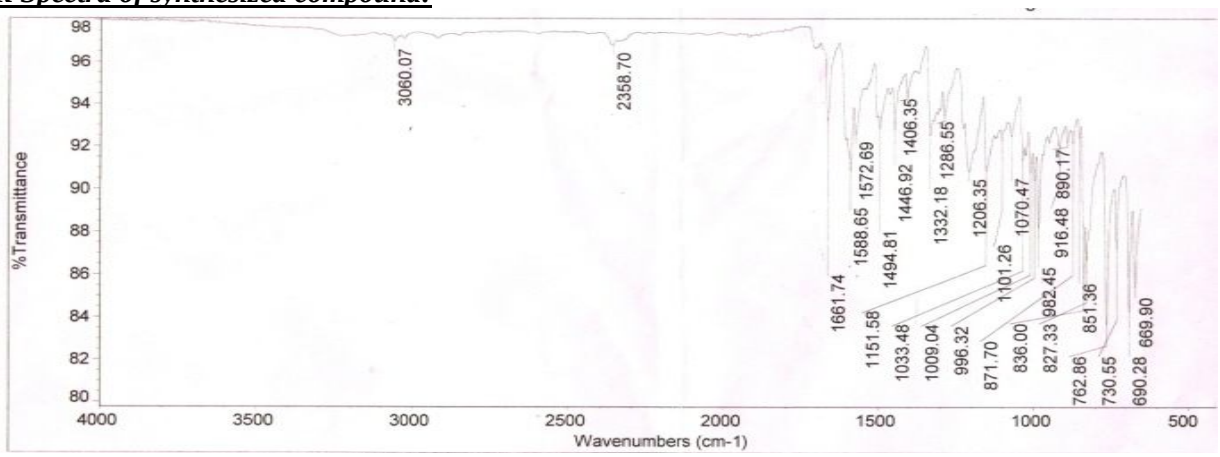
Figure 5: Relation between Free Energy and % composition of methanol

Table 2: Thermodynamic parameters of 4'-Fluorochalcone in methanol + benzene mixtures

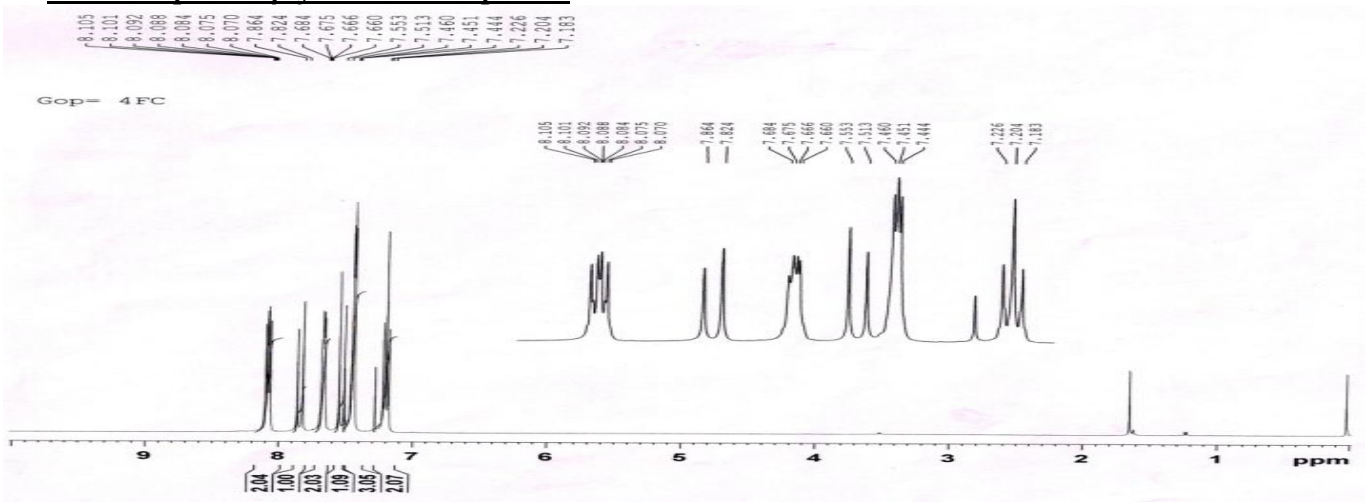
Wt.% of methanol	Effective Molecular Weight (M_{eff})	Wada's constant (W) $\times 10^{-3}$	Absorption coefficient $\left(\frac{\alpha}{f^2}\right) \times 10^{-5}$ $m^{-1}s^2$	Viscous relaxation time (τ) $x10^{-7}$ s	Solvation Number (Sn) $x10^6$	Gibb's Free Energy $(\Delta G) \times 10^{-7}$ J/mole
0	78.000	109.08	1.5436	7.8280	31.120	- 4.9977
10	68.900	99.531	2.2450	10.743	27.489	- 4.4938
20	61.587	26.036	2.3162	11.387	24.573	- 4.4011
30	55.578	73.563	2.4081	11.746	22.174	- 4.3517
40	50.555	66.055	2.4580	12.212	20.169	- 4.2897
50	46.293	60.297	2.4665	12.465	18.469	- 4.2571
60	42.628	55.523	2.5024	12.690	17.007	- 4.2286
70	39.447	50.275	2.5645	13.005	15.738	- 4.1896
80	36.660	46.925	2.5943	13.156	14.626	- 4.1712
90	34.194	43.345	2.6000	13.184	13.642	- 4.1679
100	32.000	40.046	2.6409	13.393	12.767	- 4.1428

Spectras of synthesized compounds:

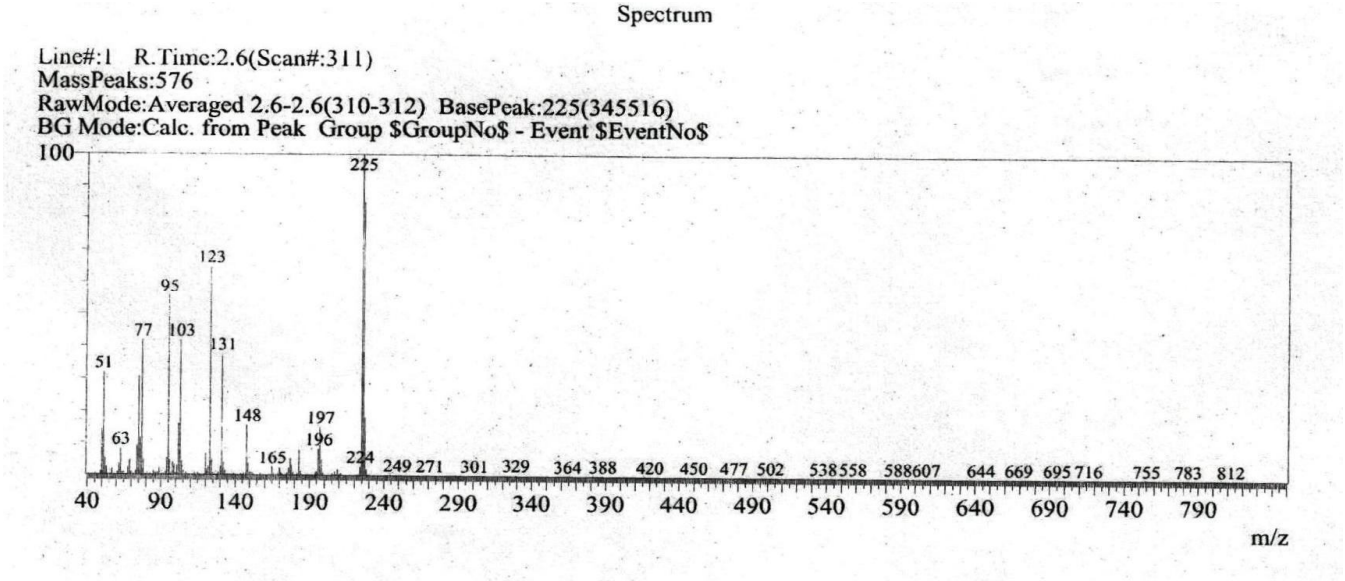
IR Spectra of synthesized compound:



H1NMR Spectra of synthesized compound:



Mass Spectra of synthesized compound:



CONCLUSION

The acoustical parameters gives valuable information to understand the solute-solvent interactions in the binary solvent system; it showed that molecular interactions resulted in structure forming as judged on the basis of positive values of solvation number.

The studied various thermodynamic parameters supports the existence of weak and strong dispersive forces in this binary mixtures.

ACKNOWLEDGEMENT

Authors are thankful to In-charge, Computer science department Shivaji University, Kolhapur and In-charge Instrumentation Department Solapur University, Solapur for providing facilities for the characterization of the sample.

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