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Effect of Dioxane on *N*-(4-hydroxy-6-methyl-1,3,5-triazin-2-yl)-*N*'-phenylthiocarbamide

D. T. Tayade[1] and A. M. Kshirsagar[2,*]

[1]*Department of Chemistry, Government Institute of Science and Humanities, Amravati, PIN 444 604, S.G.B. Amravati University, (M.S.), India;* [2]*Department of Chemistry, Alamuri Ratnamala Institute of Engineering and Technology, Sapgaon, Taluka-Shahapur, Dist.-Thane (M.S.), Mumbai University, (M.S.), India*

Abstract: In present times, the drugs containing S-triazino and thiocarbamido nucleus created their own identity and importance in medicinal, pharmaceutical and industrial fields due to their ability of curing wide range of diseases caused by various pathogens. These types of drugs showed remarkable and noticeable antibacterial, antifungal and antiviral activities. Hence, viscometric, refractrometric and interferometric measurements of recently synthesized compound have been investigated at 25°C in 60% dioxane-water system at various concentrations. The results obtained in these studies evidently explain polarizability, mutual compensation of dipoles and solute-solvent interactions. The values of acoustic parameters are useful for cross justification of solute-solvent interactions. These results are most indispensable for knowing the pharmacokinetics and pharmacodynamics of any drug. An absorption, transmission, metabolism and excretion of any drug depend on solute-solvent, solute-solute-solvent and solute-solvent-solvent interactions, taking all these things into consideration this research work was carried out.

Keywords: Viscometric, refractrometry and interferometric measurements, pharmacokinetics and pharmacodynamics.

INTRODUCTION

The medicinal field is undefined without heteroacycles and heterocycles. Most of the drugs contain heteroacyclic and heterocyclic nucleus having their meticulous medicinal and pharmaceutical properties. The S-triazino compounds initiate the new branches of development in the medicinal, pharmaceutical, agricultural, biochemical and industrial fields [1,2]. The drugs containing S-triazino nucleus are used as hypoglycemic agent, blood pressure depressant [3-6], antibacterial [2], anti-inflammatory [4] anti-psychotic agent [5]. To determine the pharmacokinetics and pharmacodynamics of any drug, in medicinal and drug chemistry, the viscometric, refractometric and interferometric measurements play an important role [7-9]. It is the prime duty of the chemist to be acquainted with drug activity and drug effect of newly synthesized drug before its biological and medicinal study. Theoretically, drug activity and drug effect can be easily determined by knowing solute-solvent interactions.

Viscometric, refractrometric and interferometric measurement methods are very useful, handy, easy and suitable for studying solute-solvent interactions. Drug activity and drug effect can be explained by knowing such types of interactions. The successful application of acoustic methods to physiochemical interactions of solution becomes possible after the development of adequate theoretical approaches and methods for precise ultrasonic velocity measurements in minimum volumes of liquids [10, 11]. Most of the information procured from ultrasonic study of fluids is confined to the determination of hydration number and compressibility [12-14]. In the basic sciences, these waves are used to provide information on the behavior of microscopic particle of matter [15]. The use of ultrasound was proved to be useful probe for generating more information on oregano metallic chemistry, biotechnology, polymerization medicinal use [16-18].

The drug is variously taken in the form of capsule, tablet or syrup. Here, drug is considered as solute and blood as a solvent. When drug is absorbed and transmitted in blood; the drug metabolism starts and at last there occurs excretion of bye-product, if formed. All systems in the body directly or indirectly take part in this process. Each step in the pharmacokinetics and pharmacodynamics depends on solute-solvent, solute-solute-solvent and solute-solvent-solvent interactions. Such types of interactions portray drug activity and drug effect theoretically. Hence, before biological testing and recognizing any synthesized compound as a drug, pharmacokinetics and pharmacodynamics of that compound must be evaluated. On the basis of this study, potency, usefulness and significance of that compound is predicted.

Therefore, for knowing the potency of *N*-(4-hydroxy-6-methyl-1,3,5-triazin-2-yl)-*N*'-phenylthiocarbamide the viscometric, refractometric and interferometric study was carried out.

MATERIALS

Carbon dioxide free, double distilled water was used. Extra pure (E. Merck) dioxane was further purified by the prescribed procedure [19] and used for the preparation of drug

*Address correspondence to this author at the Department of Chemistry, Alamuri Ratnamala Institute of Engineering and Technology, Sapgaon, Taluka-Shahapur, Dist.-Thane (M.S.), Mumbai University, (M.S.), India, Tel: +919545192107; E-mail: ashwinikshirsagar2@gmail.com

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solutions. Ostwald's viscometer was used for the determination of viscosities. *N*-(4-Hydroxy-6-methyl-1,3,5-triazin-2-yl)-*N*'-phenylthiocarbamide is as shown in Fig. (**1**) is prepared by known literature method [20].

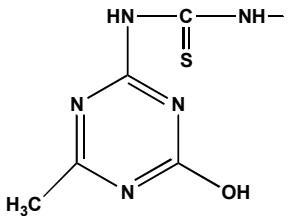

Fig. (1). 1-(4-Hydroxy-6-methyl)-S-triazino-3-phenylthicarbamide.

METHODOLOGY

The Ostwald's viscometer was kept in Elite thermostatic water bath and temperature variation was maintained at 25^0C (±0.1) for each measurements. The refractive indices of solvent mixture and solutions were measured by Abbe's refractrometer (±0.001). Initially, the refractometer was calibrated. For evaluating the molar refraction and polarizability constant of the compounds, we prepared 0.1M, 0.075M, 0.56M and 0.042M solutions in 60% dioxane-water mixture at 25˚C. The temperature was maintained by using the thermostat. The data obtained was used to compute intermolecular interactions. The refractrometric readings were taken as described in literature [19]. Single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy ±0.03% and frequency 1 MHz was used in the present work. The working of the ultrasonic interferometer was checked by measuring ultrasonic velocity of pure water at 25^0C. The measured value is in good agreement [21,22] with literature value 1484.38 ms^{-1} as shown in (Table **1**). The ultrasonic velocity was calculated in various concentrations at 25^0C in 60% dioxane-water mixture. The molecular interactions were studied with solute; the effect of this is especially related to protic-aprotic nature, polarity-non polarity and hydrogen boding in solvent. The dielectric constant, density, viscosity and surface tension of solvent on solute-solvent, ion-solvent and ion-ion interactions were also investigated during the work.

Treatment Data

The relative viscosity is calculated by,

$$\eta_r = d_s \times t_s / d_\omega \times t_\omega \quad (1)$$

Where, η = Relative viscosity.

η_r = Relative viscosity of synthesized compound solution.

d_s and d_ω= Density of synthesized compound solution and water respectively.

t_s and t_ω = Time of flow for synthesized compound solution and water respectively.

The relative viscosities have been analyzed by Jone's-Dole equation

$$(\eta_r - 1)\sqrt{C} = A + \beta\sqrt{C} \quad (2)$$

Where, **C**-is molar concentration of the synthesized compound solution.

A-is the Falkenhagen coefficient.

β-is the Jones's –Dole coefficient.

The molar refraction of solutions of synthesized compound in dioxane-water mixture were determined by a following equation,

$$R_{mixture} = [(\acute{\eta}^2 - 1) / (\acute{\eta}^2 + 2)]\{[X_1M_1 + X_2M_2 + X_3M_3]/d\} \quad (3)$$

Where,

$\acute{\eta}$ is the refractive index of solution,

X_1 is mole function of dioxane,

X_2 is mole function of water,

X_3 is mole function of solute,

M_1, M_2, M_3 are molecular weights of dioxane, water and solute respectively,

d is density of solution

The molar refraction of compound is calculated by,

$$R_{lig} = R_{mixture} - R_{dioxane\text{-}water} \quad (4)$$

Where,

$R_{dioxane\text{-}water}$ - The molar refraction of solvent, dioxane-water mixture.

Table 1. Average Ultrasonic Velocity of Water

Sr. No.	No. of Rotation of Screw	Micrometer Reading (mm)	Difference Between Reading (mm)	Distance Travelled By Screw in One Rotation	Average Ultrasonic Velocity (m/sec)
1	5	26.1245	1.5981	0.6392	1484.3828
2	10	24.5264	5.1700	2.0680	
3	15	19.3564	4.1018	1.6407	
4	20	15.2546	2.9982	1.1993	
5	25	12.2564	5.0016	2.0006	
6	30	7.2548	3.8852	1.5541	
7	35	3.3696	3.2218	1.2887	
8	40	0.1478		10.3907	

The polarizability constant (α) of compound is calculated by the following relation,

$$R_{lig} = (4/3)\ \pi\ No\ \alpha \quad (5)$$

Where, N_o is Avogadro's number. And **α** is polarizability constant.

RESULT AND DISCUSSION

The relative viscosity is determined by using Equation 1 and the results obtained are given in (Table **2**). The Fig. (**2**) is plotted in between the **√C** versus **√(η$_r$-1)/√C**. From the slope of Fig. (**2**) the values of A and β-coefficient were determined and are given in (Table **3**). The graph for this system gave linear straight line showing validity of Jone's–Dole equation.

Generally, aromatic compounds show high value of relative viscosity. In this investigation, the value of relative viscosity of compound indicates the resonance stabilization in benzene as well as S-triazino rings. These rings restrict the tautomeric changes in the thiocarbamido group. From this, it is clear that bulky substituent on the molecule is not only factor which change the trend of relative viscosity but the reactivity, stability and restriction in tautomeric conversion also influence the relative viscosity. From Table **3** the values of "A" and negative values of β-coefficient are characterized as 'structure-breaker', indicating a weak solute-solvent interactions which is the best factor for drug activity and drug effect and it favors pharmacokinetics and pharmacodynamics of drug.

The values of molar refraction of dioxane in 60% dioxane-water mixture are shown in (Tables **4** and **5**). The values of molar refraction and polarizability constant of compound in 60% of dioxane-water mixture are presented in (Table **4** and **5** clear from Fig. **3**). From the data, it can be predicted that at 25^0C temperature the molar refractivity (true molar volume) and polarizability constant of compound (α) continuously decreases with concentration. This may be attributed to the fact that at this temperature, there is a decrease in dielectric constant of the medium and considerable dipole association (intermolecular attraction) takes place. From this study it is clear that not only bulkier groups affect the molar refraction but tautomeric restrictions also affect the values of molar refraction.

An addition of polar solute, having a partial positive charge on hydrogen atom, to dioxane there is more possibility of a weak interaction between the positive charge of hydrogen atom from polar solute and negative charge on oxygen atom (due to electro negativity) of dioxane. This weak interaction of the Van der waal's forces is expected to introduce the structuredness in the solution i.e. specific arrangement of dioxane molecule may be occurring due to attached solute molecule. The results are given in (Tables **6** and **7**). Thus, spaces may be created making the solution more compressible as it appears from the higher apparent molar compressibility value in dioxane solvent. The adiabatic compressibility shows the increase association of molecules by lower β value.

$$\beta = 1/\ V_s^2 d \quad (6)$$

Table 2. Determination of Relative and Specific Viscosities

System: Compound (L)				Medium - 60% Dioxane-Water			
Temp T(°C)	**Conc. C(M)**	**√C**	**Time t (sec.)**	**Density dx10^3 (kg.cm^{-3})**	**η$_r$**	**η$_{sp}$= η$_r$ -1**	**(η$_r$-1)/√C (pa˙s)**
25	0.100	0.31623	451.98	1.0246	1.8465	0.8465	2.67687
	0.075	0.27386	428.26	1.0243	1.7491	0.7491	2.73533
	0.056	0.23664	414.00	1.0241	1.6905	0.6905	2.91790
	0.042	0.20494	398.15	1.0239	1.6255	0.6255	3.05213

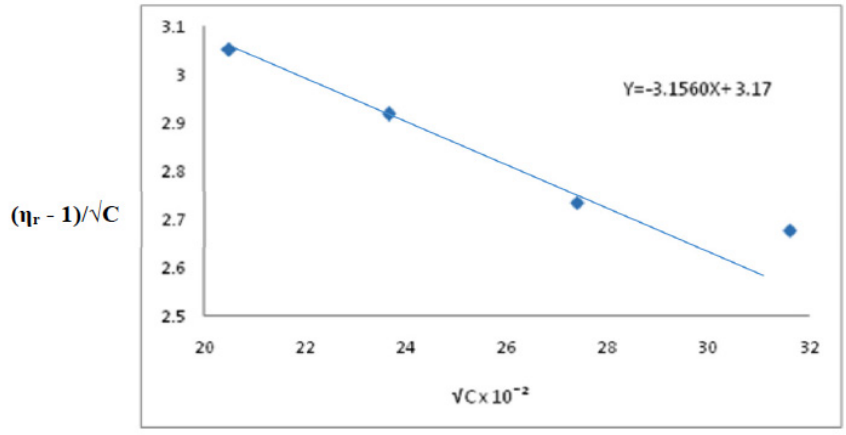

Fig. (2). Graph plotted between (η$_r$ - 1)/√C versus √C at different concentrations.

Table 3. A and β Co-efficient Value from Graphs (in Figs.)

Compound	Temp °C	Mean "A"	B (Slope "m")
L	25	3.17	-3.1560

Table 4. Molar Refraction of Different Percentage of Dioxane - Water Mixture

% of Dioxane-Water Mixture	Molar Refraction (RM) (cm^3 . $Mole^{-1}$)
100	21.5977
90	15.4584
80	11.9390
70	9.6554
60	8.0551

$$\phi_K = [1000\ (\beta_s d_0 - \beta_0 d_s) / m d_s d_0] + ((\beta s M/d_s) \quad (7)$$

Where,

M = molecular weight of solute,

β_0 = adiabatic compressibility of pure solvent and

β_s = adiabatic compressibility of solution.

d_0 = density of pure solvent

d_s = density of solution

m = molality of solution

Apparent molar compressibility also shows the increased association and at the same time the structuredness of the solution which can be observed from higher ϕ_K values. It is also observed that positive values of ϕ_K for compound indicates electrostatic force in the vicinity of ions [23,24].

$$\phi_V = [1000(d_0 - d_s) / m d_0 d_s] + (M/ d_s) \quad (8)$$

From the difference in trends of adiabatic and apparent molar compressibility it can be predicted that adiabatic compressibility detects gross changes in the interactions but minute changes due to change in structure may only be noticed by apparent molar compressibility (ϕ_K). Thus, the structure of solute and the number of atoms present in it will have direct effect on ϕ_K value clearly indicated from (Fig. **4** and Fig. **5**). High density of dioxane as compared to protic nature, polarity, high dielectric constant (24.6) directly affects the values of β. Similarly, on increasing the concentration of solute β decreases continuously. The increased concentration of solute will require more and more number of solvent molecules to dissolve it; resulting in the breaking of electrostriction of solvent which consequently decreases the compressibility. Thus, in these systems both solute-solvent and solvent-solvent interactions are involved which are reflected in the compressibility values. The conventional approach based on compressibility is useful and fundamental for studying interactions of solvent and solute. This is an additional probe for studying molecular interactions. Specific acoustic impedance is the complex ratio of the effective sound pressure at a point to the effective particle velocity at that point [25]. In dioxane the molecules are compactly packed. When polar solute is added to it then due to its association free space decreases. Therefore, the L_f values in dioxane get smaller. When the metal ions are added, the polar-polar associations still increase and the L_f decrease. Ultrasonic velocity depends upon intermolecular free length L_f. With decrease in free length; velocity increases or vice versa.

$$L_f = K.\ (\beta s)^{1/2} \quad (9)$$

Where,

L_f = Intermolecular free length

K = Jacobson's constant

Relative association R_A is an acoustic property of understanding interaction, which is influenced by two opposing factors,

$$R_A = d_s/d_0\ [V_0/V_S]^{1/3} \quad (10)$$

$$Z = V_s\, d_s \quad (11)$$

Where,

V_0 = ultrasonic velocities in a solvent.

V_s = ultrasonic velocity of solution.

It was observed that, the value of R_A of the solute gets affected by the resonance stabilization in benzene as well as in S-triazino rings. It is clearly observed from the high concentration of solute that the solvation of the solute is affected by the free solvent of molecules. The values of R_A at high percentage of dioxane are very well explained by second factor.

Hence, from the above results and discussions it can be clearly observed that there are solute-solvent and solvent-solvent interactions which are the basic and primary requirements of pharmacokinetics and pharmacodynamics of the drug. From these results the drug absorption, drug transmission, drug metabolism, drug activity and drug effect of synthesized compound can be theoretically predicted. This is

Table 5. Determination of Molar Refraction and Polarizability Constant

Temp (°C)	Concentration (M)	Density $dx10^3$ ($kg.cm^{-3}$)	Refractive Index η	R_{mix} ($cm^3.mole^{-1)}$	$R_{Compound}$ ($cm^3.mole^{-1}$)	$\alpha x10^{-23}$ (cm^3)
25	0.1000	1.0246	1.4110	8.8577	0.8026	0.03180
	0.0750	1.0243	1.4102	8.7976	0.7425	0.02942
	0.0560	1.0241	1.4098	8.7556	0.7005	0.02776
	0.0420	1.0239	1.4088	8.7059	0.6508	0.02579

Table 6. Average Ultrasonic Velocity of Dioxane (β_0)

D-W %	Sr. No.	No. of Rotation of Screw	Micrometer Reading (mm)	Difference Between Reading	Distance Travelled By Screw in One Rotation	Average Ultra-sonic Velocity (v_0) (m/sec)	Density (d_0) ($Kg.m^{-3}$)	$\beta_0 \times 10^{-10}$ (Pa^{-1})
25˚C	1	5	19.6584	3.4029	1.3617	1442.7	1027.3	4.6768
	2	10	16.2555	3.9301	1.5720			
	3	15	12.3254	3.9558	1.5823			
	4	20	8.3696	3.1382	1.2553			
	5	25	5.2314					
					5.7708			

Table 7. Acoustic Parameters at Different Concentration of Compound L

Temp.	Conc. C (Mole/lit)	Average Ultra-sonic Velocity V (m/sec)	Density d_s ($Kg.m^{-3}$)	$\beta s \times 10^{-10}$ (pa^{-1})	ϕ_v (m^3mol^{-1})	$\phi_k \times 10^{-10}$	L_f (A_0)	R_A	$Z * 10^4$ ($Kgm^{-2}sec^{-1}$)
25˚C	0.1	1612.59	1024.6	3.7532	0.2804	-7.9387	0.0122	0.9610	165.2260
	0.075	1509.366	1024.3	4.2853	0.2833	-3.8264	0.0131	0.9822	154.6043
	0.056	1388.022	1024.1	5.0683	0.2853	8.3725	0.0142	1.0098	142.1473
	0.042	1192.682	1023.9	6.8658	0.2872	53.0128	0.0165	1.0620	122.1187

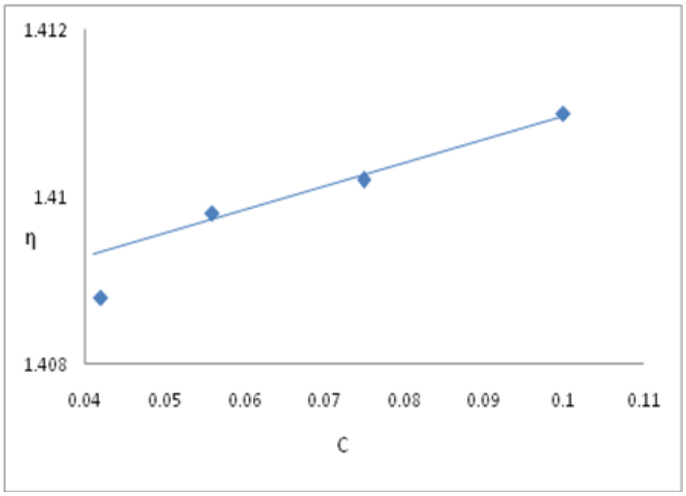

Fig. (3). Graph plotted between refractive index (η) versus C at different concentrations.

the prime and basic requirement of pharmaceutical and drug chemistry.

CONCLUSION

In general, it is observed that the values of β, ϕ_v, L_f of newly synthesized compound clearly indicate the effects of resonance stabilization in benzene and S-triazino rings which are substituent on thiocarbamido nucleus. These rings restrict tautomeric changes in thiocarbamido group.

From this study it was observed that the bulkier nature of substituent, resonance in the molecule, tautomeric conversion and nature of solute and molecular weight of solute are important factors which directly affect the solute-solvent interactions. The solvent-solvent and solute-solvent interactions are also governed by density of dioxane and water, viscosity of the solution, protic nature, polarity, dielectric constant which directly affect the values of β. Similarly, on increasing the concentration of solute, the change in values of L_f may be due to stronger interactions between ions and solvent molecules at that particular percentage combination of dioxane-water mixture whereas, decrease in L_f values indicated weaker interactions between ions and solvent

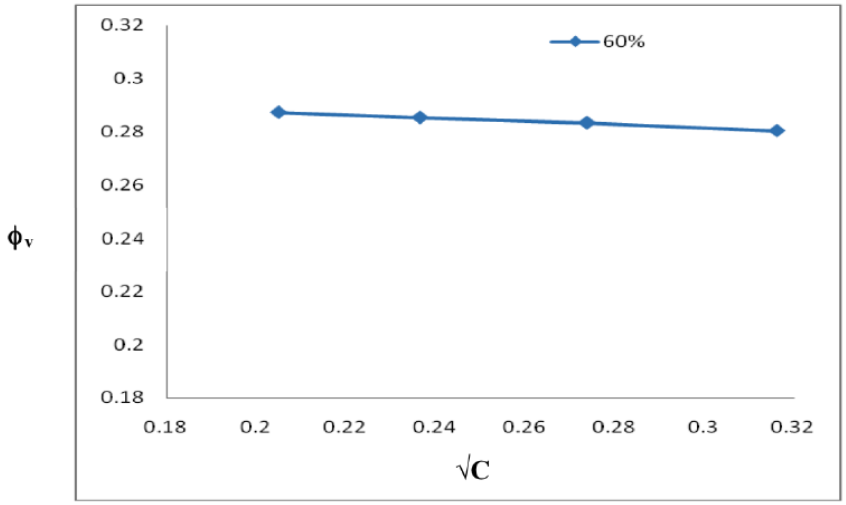

Fig. (4). Plot between apparent molar volume (ϕ_v) Vs concentration (√C) for ligand L.

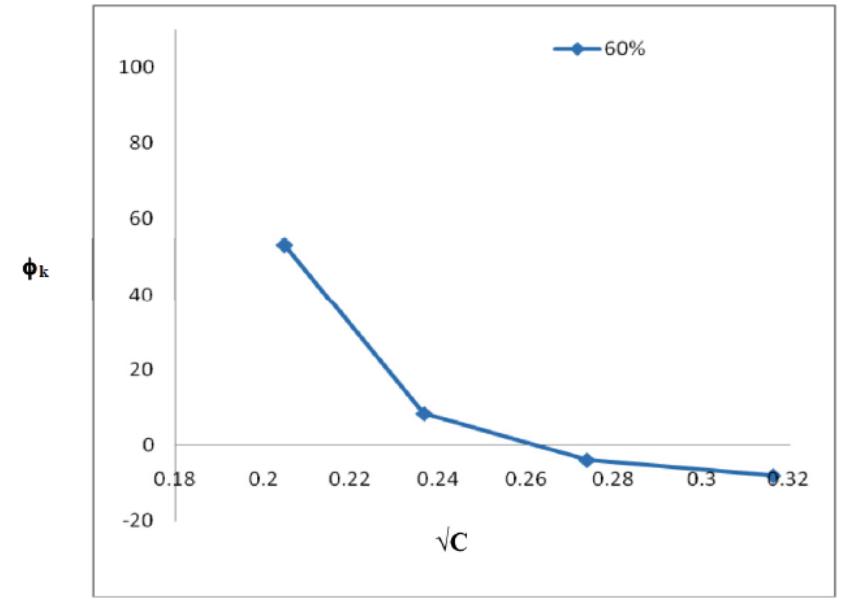

Fig. (5). Plot between apparent molar compressibility (ϕ_k) Vs concentration (√C) for ligand L

molecules. The intermolecular free length goes on decreasing with increase in concentration of solute which indicates decrease in free space between the molecules because of stronger solute-solvent interactions which is in agreement with on observed value of β.

Measurement of ultrasonic velocity is the best tool to investigate solute-solvent, solute-solute and ion-solvent interactions. Therefore, from the last four decades ultrasonic interferometric study has established its own identity and importance for determining solute-solvent interactions. From this study, acoustic properties viz; β, ϕ_v, ϕ_K, L_f, R_A, and Z, which explain how these interactions occur and are responsible for breaking and making of the structure in the solution, can be determined. So, in the present work these acoustic parameters were studied for newly synthesized Compounds, which were used as solutes.

The three techniques used for this study require minimum solutions, are non destructive, easy to handle, have low maintenance and do not require electricity. The results obtained are accurate. So, these techniques are creating their own identity and significance in material sciences.

This study is an important and basic tool for pharmaceutical, medicinal and biochemical sciences which directly predict drug activity and drug effect at primary level by knowing the solute-solvent, solute-solute and ion-solvent interactions which is most essential to determine the characteristics of the drug before its antimicrobial, biological, physiological and anatomical study on living beings and human beings. This study intended to give detailed information regarding pharmacokinetics and pharmacodynamics of the synthesized compound.

CONFLICT OF INTEREST

The author(s) confirm that this article content has no conflicts of interest.

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