ACOUSTIC STUDY OF S-SUBSTITUTED TRIAZINOTHIOCARBAMIDES IN 70 % DIOXANE WATER MIXTURE

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Abstract:

In last four decades, S-triazine and thiocarbamide group containing drug create their own identity in the drug, pharmaceutical and medicinal sciences. The Interferometric measurements of recently synthesized drug have been carried out for solutions of 1-(4-hydroxy-6-methyl)-S-triazino-3-phenylthiocarbamide (L_1) at various concentrations. The result obtained during this investigation directly through light on the dipole association of compound, intermolecular attraction between solute and solvent, dielectric constant of medium, polarizability and mutual compensation of dipoles, various acoustic/ thermodynamic parameters and useful for drug absorption, transmission, stability, activity and effect of these on drugs which is base of pharmacokinetics and pharmacodynamics of any drug.

Keywords:

Acoustic parameters, 1-(4-hydroxy-6-methyl)-S-triazino-3-phenylthiocarbamide (L_1), Interferometric measurements.

Introduction:

In the recent era, the heterocycles and drugs are both interconnected with each other. Most of the modern drugs contain heterocyclic nucleus[1,2]. The S-triazino compounds initiated the new branches of development in the medicinal[3,4] pharmaceutical, agricultural and biochemical fields[5-7] and used as drugs as hypoglycemic agent[3], blood pressure depressant[4] anti-tumor properties[8], anti-bacterial[2,9], anti-inflammatory[6], antipsychotic agent[7], herbicidal[10,11], insecticidal.[12-15]

The result obtained during this investigation directly through light on the dipole association of compound, intermolecular attraction between solute and solvent, dielectric constant of medium, polarizability, and mutual compensation of dipoles and useful for transmission, stability, activity and effect of drug. Most of the information procured from ultrasonic study of fluids is confined to the determination of hydration number and compressibility[16-18].. Drug receptors are the enzymes and directly hamper the drug activity and drug effects. It makes direct or indirect physical and chemical reactions with drug i.e. solute-solute interactions in the presence of solvent which changes viscosity of the phase during drug action and before testing and applying that drug to the patients, drug activity and drug effect must be evaluated. S-triazino and thiocarbamido nucleus containing drugs create its own identity and significance in the medicinal, drug[19-21] and pharmaceutical chemistry[22-25].

Hence for studying the potency of recently synthesized drugs in this laboratory, the interferometric measurements of 1-(4-hydroxy-6-methyl)-S-triazino-3-phenylthiocarbamide (L_1)) was studied at 35°C temperature .

Experimental:

Materials and Solutions

Extra pure (E. Merck) dioxane was further purified by the prescribed procedure and used for preparation of ligand solutions. The entire chemical used of A.R. grade. All weighing were made on Mechaniki Zaktady Precyzying Gdansk Balance Poland make, (±0.001g). The density of solutions were determined by a bicapillary Pyknometer (±0.2%) having a bulb volume of about 10 cm^3 and capillary having an internal diameter of 1mm and calibrated with deionised doubly distilled water. The accuracy of density measurements were within ±0.1Kgm^{-3}. 1-(4-hydroxy-6-methyl)-S-triazino-3-phenylthiocarbamide (L_1). 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 35^0C with literature value 1512 ms^{-1} as shown in **Table No.I.**

Observations and Calculations:

The adiabatic compressibility shows the increase association of molecules by lower β value.

$$\beta = 1/ V_s^2 d \qquad \text{…….. 1}$$

$$\phi_K = 1000 (\beta_s d_0 - \beta_0 d_s) / m d_s d_0 + ((\beta_s M/d_s) \qquad \text{…….. 2}$$

Whereas, apparent molar compressibility also shows in **Table No I and II.** The increase association but at the same time the structuredness of the solution by higher ϕ_K values. It is also observed from the graphs that positive values of ϕ_K for ligands indicates electro static force in the vicinity of ions[43,44].

$$\phi_V = 1000(d_0 - d_s) / m d_0 d_s + (M/ d_s) \quad \text{..... 3}$$

$$L_f = K. (\beta_s)^{1/2} \quad \text{..... 4}$$

$$R_A = d_s / d_0 \, V_0/V_S^{1/3} \quad \text{..... 5}$$

$$Z = V_s d_s \quad \text{..... 6}$$

By this study β, ϕ_v, ϕ_K, L_f, R_A, Z, etc. acoustic properties were determined which explain how these interactions occur and responsible for breaking and making of the structure in the solution. The change in values of L_f may be due to stronger interaction between ions and solvent molecules at that particular percentage combination of dioxane-water mixture decrease in L_f values indicated weaker interaction between ions and solvent molecules. The intermolecular free length goes on decreasing with increase in concentration of solute indicates decrease in free space between the molecules because of stronger solute-solvent interaction which is in a agreement with on observed value of β.

Table:

Table No. I : Average Ultrasonic Velocity of Water at 35˚C

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	26.8954	3.77	1.508	1512.7943
2	10	23.1254	3.7596	1.5038	
3	15	19.3658	4.1293	1.6517	
4	20	15.2365	4.0019	1.6008	
5	25	11.2346	2.9782	1.1913	
6	30	8.2564	3.9308	1.5723	
7	35	4.3256	3.9041	1.5616	
8	40	0.4215		10.5896	

Table No. II: Average Ultrasonic Velocity of Dioxane at 35˚C (β_0)

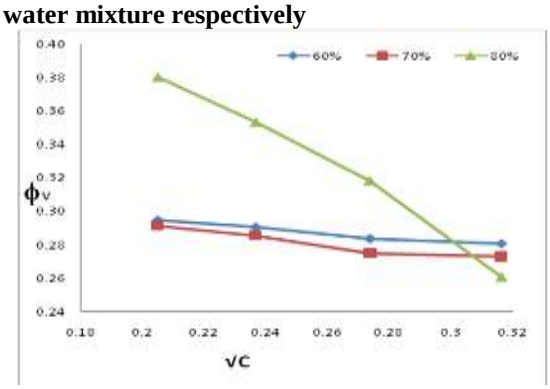
D-W %	Sr. No.	No. of Rotation of Screw	Micrometer Reading (mm)	Difference Between Reading	Distance Travelled By Screw in One Rotation	Average Ultrasonic Velocity (v_0) (m/sec)	Density (d_0) ($Kg.m^{-3}$)	$\beta_0 \times 10^{-10}$ (Pa^{-1})
70	1	5	17.1258	3.8603	1.5441	1466.9	1030	4.5119
	2	10	13.2655	3.6130	1.4452			
	3	15	9.6525	3.6330	1.4532			
	4	20	6.0195	3.5627	1.4251			
	5	25	2.4568					
					5.8676			

Table No. III: Acoustic Parameters at Different Concentration of Ligand L_1 at 35˚C

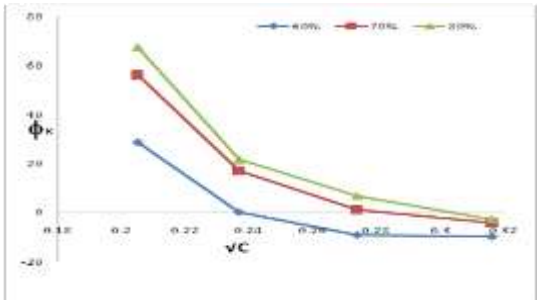
D-W %	Conc. C (Mole/lit)	Average Ultrasonic Velocity V (m/sec)	Density d_s ($Kg.m^{-3}$)	$\beta s x10^{-10}$ (pa^{-1})	ϕ_V (m^3mol^{-1})	ϕ_k $x10^{-10}$	L_f (A_0)	R_A	$Z * 10^4$ ($Kgm^{-2}sec^{-1}$)
70	0.1	1564.755	1029	3.9691	0.2728	-4.1875	0.0126	0.9778	161.0133
	0.075	1468.93	1028.8	4.5047	0.2747	1.1754	0.0134	0.9984	151.1235
	0.056	1343.11	1026.7	5.3992	0.2854	17.0570	0.0147	1.0265	137.8971
	0.042	1193.578	1026.1	6.8408	0.2913	56.1761	0.0165	1.0671	122.4730

Graph:

Plot Between Apparent molar volume (ϕ_v) Vs concentration ($\sqrt{C}$) for Ligand L_1 at 35^0Cat 70% dioxane-water mixture respectively



Plot between Apparent molar compressibility (ϕ_k) Vs concentration ($\sqrt{C}$) for Ligand L_1 at 35^0C at 70% dioxane-water mixture respectively



Conclusion:

Hence from all three method , it was clear that bulky substituent on the molecule was not only factor in trend but tautomeric conversion as well as electron donating nature, electron clouds, nature of hetero atom present in compounds and compactness in the molecule will directly hampered results and trends. It means that in 70% of dioxane, the solute-solvent interactions i.e. interaction of compounds (drugs) and dioxane is more but phenyl substituted drug shows more reactivity as compare to other substituent, which may affect the drug activity in dioxane as medium. By every method it is proved.

From this study it can be concluded that interferometric technique requires minimum efforts, solutions and is somewhat a direct method as compare to other two and has its own identity and significance in material sciences, which can give idea about effectiveness of solvent. By knowing these parameters the selection of solvent during synthesis in organic and coordination chemistry can be predicted. This study is an important

basic tool for pharmaceutical, medicinal and biochemical sciences which directly focus on drug activity and drug effect at primary level and then onwards only the characteristics of drug can be decided. This study gave detail information regarding pharmacokinetics and pharmacodynamics of drug.

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