



Acoustic Study of S-Substituted Triazinothiocarbamides

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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 (L₁) 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 (L₁), Interferometry measurements.

1. 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 fields⁵⁻⁷ and used as drugs as hypoglycemic agent³, blood pressure depressant⁴ anti-tumor properties⁸, anti-bacterial^{2,9}, anti-inflammatory⁶, antipsychotic agent⁷, herbicidal^{10,11}, insecticidal¹²⁻¹⁵.

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 compressibility¹⁶⁻¹⁸. 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, drug¹⁹⁻²¹ and pharmaceutical chemistry²²⁻²⁵.

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 (L₁) was studied at 35°C temperature.

2. EXPERIMENTAL

2.1 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, (± 0.001 g). The density of solutions were determined by a bicapillary Pyknometer ($\pm 0.2\%$) having a bulb volume of about 10 cm³ and capillary having an internal diameter of 1mm and calibrated with deionised doubly distilled water. The accuracy of density measurements were within ± 0.1 Kgm⁻³. 1-(4-hydroxy-6-methyl)-S-triazino-3-phenylthiocarbamide (L₁). Single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy $\pm 0.03\%$ 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°C 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.



$$\beta = 1/V_s 2d \quad \dots\dots\dots 1$$

$$\phi_K = 1000 (\beta_s d_0 - \beta_0 d_s) / m d_s d_0 + ((\beta_s M/d_s) \quad \dots\dots\dots 2$$

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}.

$$\phi_v = 1000(d_0 - d_s) / m d_0 d_s + (M/d_s) \quad \dots\dots\dots 3$$

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

$$R_A = d_s / d_0 V_0 / V_s^{1/3} \quad \dots\dots\dots 5$$

$$Z = V_s d_s \quad \dots\dots\dots 6$$

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			

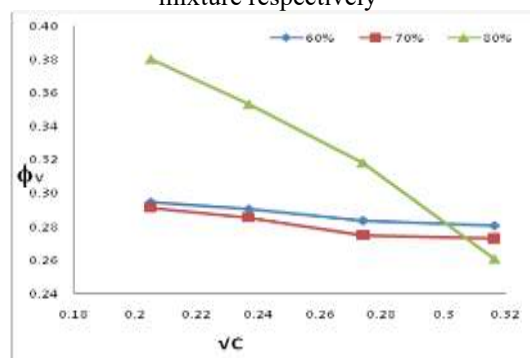
Table No. III: Acoustic Parameters at Different Concentration of Ligand L_1 at 35°C

D-W %	Conc. C (Mole/lit)	Average Ultrasonic Velocity V (m/sec)	Density d_s (Kg.m^{-3})	$\beta_{sx} 10^{-10}$ (Pa^{-1})	ϕ_v ($\text{m}^3 \text{mol}^{-1}$)	$\phi_K \times 10^{-10}$	L_f ($\text{\AA}$)	R_A	$Z \times 10^4$ ($\text{Kg m}^{-2} \text{sec}^{-1}$)
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

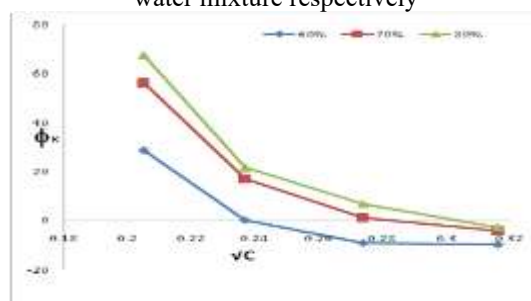


2.2 Graph

Plot between Apparent molar volume (ϕ_v) Vs concentration ($\sqrt{C}$) for Ligand L₁ at 35°C at 70% dioxane-water mixture respectively



Plot between Apparent molar compressibility (ϕ_k) Vs concentration ($\sqrt{C}$) for Ligand L₁ at 35°C at 70% dioxane-water mixture respectively



3. CONCLUSION

Hence from all three methods, it was clear that bulky substituent on the molecule was not only a 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 hamper 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 compared to other substituent, which may affect the drug activity in dioxane as a 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 compared to other two and has its own identity and significance in material sciences, which can give an idea about the 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 a primary level and then onwards only the characteristics of drug can be decided. This study gave detailed information regarding pharmacokinetics and pharmacodynamics of drug.

4. REFERENCE

- [1] Nitha B, Strayo D, Adikari S, Devasagayam T and Janardhanan K, *Evaluation of free radical scavenging activity of morel mushroom, Morchella esculenta mycelia: A potential source of therapeutically useful antioxidants*, J Pharm Biology, 2010. **48**(4): pp. 453
- [2] Yang J, Tian Y, Yang Z and Zhang T, *Effect of melamine on potassium currents in rat hippocampal CA1 neurons*, Toxicology in Vitro, 2010. **24**(2); pp. 397
- [3] Srinivas K, Srinivas W, Bhanuprakash K, Harkishore K, Murthy K, Jayathirtha U and Rao V, *Synthesis and antibacterial activity of various substituted s-triazines*, Eur J Med Chem, 2006. **41**(11): pp. 1240
- [4] Adebisi A, Koekemoer T, Adebisi A and Smith, N, *Differential effects of natural product microtubule stabilizers on microtubule assembly: single agent and combination studies with taxol, epothilone B and discodermolide*, J Pharm Biology, 2009. **47**(4): pp. 320
- [5] Frankenburg, Frances R, Baldessanini, Ross J and Neurosyphilis, *Malaria, and the Discovery of Antipsychotic Agents*, Harvard Review of Psychiatry, 2008. **16**(15), pp. 299
- [6] Krauth F, Dalise H M, Ruttinger H and Erobberg P, *Synthesis and characterization of novel 1, 2, 4-triazine derivatives with antiproliferative activity*, Bioorganic and Medicinal Chem, 2010. **18**(5): pp. 1816