

Solvation Effect of 1(4-Tolyl)-2(Phenyl Thiocarbamido)-1-Ethanol studied by Viscometrically

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ABSTRACT:

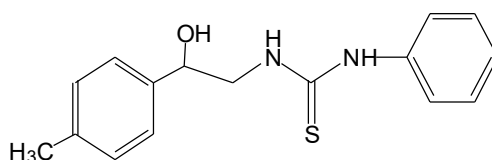
Thiocarbamide and their substituted derivatives moieties received more attention of many researchers because of their significances, especially those with thiocarbamido and substituted thiocarbamido derivatives nucleus, are noteworthy for their diverse applications in the disciplines of medicine, biochemistry, biotechnology, and pharmacology. Recently, we evaluated the density and studied the viscometric properties of 1(4-Tolyl)-2(Phenyl thiocarbamido)-1-Ethanol in our lab. This study's evaluation was conducted at various temperatures while maintaining a consistent concentration. The effects of solvent dilution and the drug's solute-solvent interaction in the present are determined by the experimental results. The findings demonstrated that when temperature rises, relative viscosity falls, indicating stronger solvation effects. The physicochemical behavior of chalcone derivatives is better understood thanks to this research, which advances medicinal science and helps create pharmaceuticals that work better.

Keywords: Solute-solvent interaction, Temperature Effects, Density Measurements, Solvation Effects, Viscometric study, 1(4-Tolyl)-2(Phenyl thiocarbamido)-1-Ethanol

1. INTRODUCTION

Thiocarbamido moiety received attention of many researchers. Heterocyclic compounds are found in nature and have attracted a lot of attention from scientists in a variety of fields because of their biological activities and wide range of applications. The heterocyclic compound with thiocarbamido nuclei and their substituted derivative is an important part of their chemical reactivity and biological activity. These substances function as the building blocks for several heterocyclic derivatives, which can be found in both natural and artificial substances. Heterocyclic molecules with substituted thiocarbamido nuclei are frequently used in pharmacological, biological, medical, and biotechnological fields [8-9]. Living organisms require heterocyclic compounds made of nitrogen and sulfur. These compounds are vital to numerous biological systems and processes. They exist in a variety of ring configurations. The presence of nitrogen and sulfur atoms in these rings gives them unique chemical properties and reactivity profiles, which are essential for their biological functions¹⁻³. Measurements of viscosity are important. Viscosity is a fundamental property of liquids that describes how resistant they are to flow. It measures how resistant a liquid is to the layers shifting in respect to one another. This resistance is brought about by internal friction that develops as the liquid's molecules move and interact with one another⁶. There are interactions between the solute and the solvent in both aqueous and non-aqueous solutions. Measurements of viscometric parameters provide this important information. A drug's behavior, including absorption, transmission, and effects, will be directly influenced by measurements of its viscosity and interactions with solvents in the human body⁴⁻⁹. These are shown to be beneficial in the treatment of cancer. Additionally, these substances showed anti-tuberculostatic, anti-HIV, anti-helminthic, antifungal, antiviral, and antibacterial qualities¹⁰⁻¹². Lubricating oil also contains substituted thiocarbamidone which effectively prevents copper corrosion¹³⁻¹⁴.

Additionally, interesting systems are water and alcohol mixes due to their complex dynamics, which are brought on by the presence of hydrogen bonds and hydrophobic groups. The fact that these mixtures are widely utilized as solvents and have thus been the subject of in-depth theoretical and experimental research adds to their significance. The viscosity of a liquid can be affected by a wide range of variables, such as temperature, size, molecular weight, intermolecular interactions, and the presence of pollutants. The assessment of viscosity facilitates comprehension of the molecular interactions and properties of binary and ternary liquid systems. Be aware that advantageous interactions may cause the viscosity of these systems to increase. Understanding density is essential as it enables one to forecast whether a substance will float or sink in a liquid. To be more specific, objects with densities less than the liquids will float in it. Moreover, it is an essential physical property that is used to ascertain the acoustic and physical properties of a substance, such as its surface tension, molar refraction, boiling temperature and dipole moment¹⁵⁻¹⁸. Several researchers¹⁹⁻²² have also studied solute-solvent interactions at different concentrations by calculating β -coefficient. Lot of efforts had been made to study viscosities of binary liquid mixtures, but no result came forward to show ideal behavior of drugs in vivo. A survey of the literature indicates that chalcone derivatives possess a wide range of pharmacological and biochemical characteristics, such as those of mydriatic, anesthetizing, antiviral, antibacterial, and anti-inflammatory drugs. The substituted thiocarbamido nucleus heterocyclic molecule finds numerous uses in the domains of medicine, biochemistry, biotechnology, and pharmaceuticals. These substances have anti-tuberculostatic, anti-viral, anti-fungal, anti-helminthic, and antibacterial properties. Furthermore, substituted thiocarbamido derivatives and dithiazines have shown promise in the treatment of cancer. This makes viscometric measurements of 1(4-Tolyl)-2(Phenyl thiocarbamido)-1-Ethanol extremely significant at varied in temperature. All things considered, this kind of research advances the field of drug science and helps create pharmaceutical goods that are more dependable and successful, improving patient outcomes in the process.



1(4-Tolyl)-2(Phenylthiocarbamido)-1-ethanol

2. EXPERIMENTAL DETAILS

All chemicals utilized in this study were of analytical grade, All investigations used double-distilled water and analytical grade (A.R.) chemicals. The compound weights were measured using a Mechaniki Zektady Precyzyjnej Gdansk balance, which has a precision of ± 0.001 grams. An Ostwald viscometer was used to measure the viscosity of liquids at a constant temperature of 29°C ($\pm 0.1^\circ\text{C}$), which was maintained using an Elite thermostatic water bath. The density measurements were conducted using a bicapillary tube with an internal diameter of 1 mm. The viscometer and the water bath were allowed enough time to reach thermal equilibrium before any measurements were made. A 60% ethanol-water system was used for the viscometric analysis of 1(4-Tolyl)-2(Phenyl thiocarbamido)-1-Ethanol at 0.1M concentration at various temperatures. Newly developed solutions were used for the evaluation. Viscometry readings were acquired in compliance with the literature²³⁻²⁵.

3. RESULTS AND DISCUSSION

The relative viscosity was calculated using the formula below..

$$\eta_r = D_s \times t_s / D_w \times t_w.$$

While Jones-Dole equation was used to examine the relative viscosities,

$$(\eta_r - 1)/\sqrt{C} = A + B\sqrt{C}$$

Where,

A = Falkenhagen coefficient

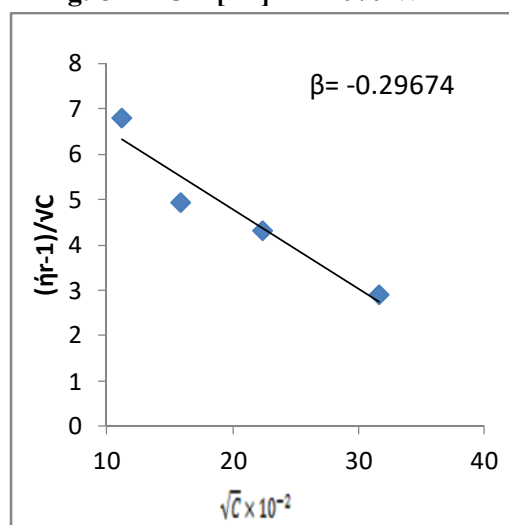
B = Jones-Dole coefficient

C = concentration of solutions

The solute-solute interaction was measured using the Falkenhagen coefficient (A), and the solute-solvent interaction was measured using the Jones-Dole coefficient (B). The graph is plotted between $(\eta_r - 1)/\sqrt{C}$ and $\sqrt{C}$. The graph of every system showed a linear straight line with a value for the β -coefficient.

Observation table-1 reveals that temperature increases time of movement of solution decreases and density decrease. Lowest relative viscosity found at 30°C and highest relative viscosity at 22°C. Along the temperature increases from 22°C to 30°C decrease in relative viscosity and specific viscosity. When graphs are plotted in between $(\eta_r - 1)/\sqrt{c}$ versus $\sqrt{c}$, they give straight line which authenticated Jones-Dole equation. Slope of straight line is β -coefficient and form intercept of that line, A can be found. 'A' which is measure of ion-ion i.e. solute-solute interactions and ' β ' which is measure of solute-solvent interactions

Fig.-32- FOR [L4] AT 70% W-E



OBSERVATIONS AND CALCULATIONS

Using the information gathered from our study, molecular interactions are expressed in terms of the β -coefficient of the solute. The collected findings are shown in Table No. 1. According to Jones-Dole equation, at different temperatures and a concentration of 0.1 M, $(\eta_r - 1)/\sqrt{C} = A + B\sqrt{C}$. Table No. 2 lists the calculated values of the A and β -coefficients.

TABLE No.1 Measurements Of Viscosity At Constant Concentrations And The Identification Of Relative And Specific Viscosities At Various Temperatures At 0.1 M.

MEDIUM - 60% ETHANOL-WATER							
Conc.	Temp. (°C)	$\sqrt{C}$	Time	Density $\rho \times 10^3$ (kg.cm ⁻³)	η_r	$\eta_{sp} = \eta_r - 1$	$(\eta_r - 1)/\sqrt{C}$ (pa-s)
0.1 M	22	0.314	61	1.101	0.082711	-0.917289	-2.921302
	24	0.314	54	1.0932	0.069965	-0.930035	-2.961894

28	0.314	49	1.0865	0.062893	-0.937107	-2.984417
30	0.314	36	1.0698	0.058637	-0.941363	-1.081363

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TABLE No.- 2

Co-efficient values of A and β for 60% as shown in the graphs. Regarding 1(4-Tolyl)-2(Phenyl thiocarbamido)-1-Ethanol.

W-E Mixture (%)	Temp° C	Mean "A"	β (Slope "m")
70	24	-2.9674	0.0071

CONCLUSION

As the temperature rises, the density and relative viscosity in the current work monitor decrease. This is supported by the observation that the solvation effect increases with temperature due to an increase in the solute-solvent interaction. Pharmacodynamic and pharmacokinetic studies are useful for scientific research and public education.

positive value of β -coefficient of viscosity reveals that strong solute-solvent interaction and termed as 'structure former'. When there is formation of hydrogen bonding in a solution then depending on situation structure formation or structure breaking occurs due to decrease or increase in interactions of solute-solvent this is due to changes in density or viscosity causing hydrophilic (structure breaking) or hydrophobic (structure making) character of solute.

Along increasing temperature intermolecular interaction decrease as a result molecule move faster over each other as a result viscosity decreases.

Lower viscosity factor supportive for the movement of molecules or drugs. That is important and support for the transmission or diffusion of the drugs molecules that will be contributed for good pharmacodynamic and pharmacokinetics of the drugs molecules. After the metabolism of drugs ions get start to move toward target lower viscous molecular solution have good diffusion activity.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests.

ACKNOWLEDGEMENTS

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