NOTE

Studies on Solute-Solvent Interactions between Substituted Isoxazolines and Different Percentages of Dioxane-Water and Methanol-Water Mixture

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The present study deals with the study of molecular interactions in terms of viscosity β-coefficient of ligands such as 3-(5-chloro-2-hydroxyphenyl)-5-phenyl-Δ^2-isoxazoline (L_1), 3-(3-bromo-5-chloro-2-hydroxyphenyl)-5-phenyl-Δ^2-isoxazoline (L_2) and 3-(5-chloro-2-hydroxy-3-nitrophenyl)-5-phenyl-Δ^2-isoxazoline (L_3) in 70, 75, 80, 85% percentage of dioxane-water and methanol-water mixtures.

Key Words: Solute-Solvent Interactions, Viscosity, Substituted isoxazolines, Dioxane-Water mixture.

The solute and solute-solvent interactions have been studied in aqueous and non-aqueous solutions by various workers[1-11]. The present study deals with the study of molecular interactions in terms of viscosity β-coefficient of isoxazoline ligands such as 3-(5-chloro-2-hydroxyphenyl)-5-phenyl-Δ^2-isoxazoline (L_1), 3-(3-bromo-5-chloro-2-hydroxyphenyl)-5-phenyl-Δ^2-isoxazoline (L_2), 3-(5-chloro-2-hydroxy-3-nitrophenyl)-5-phenyl-Δ^2-isoxazoline in 70, 75, 80, 85% percentage of dioxane-water and methanol-water mixtures.

The ligands were prepared by the standard procedure. Reagent grade dioxane and methanol (BDH, India) were purified by the procedure recommended by Vogel. Solutions of ligands in various percentages of dioxane-water and methanol-water were prepared by weight within an accuracy of 0.2 mg. The densities of water and solution were determined by pyknometer. The viscosities were measured by means of Canon Fenske viscometor at $30 \pm 0.1\,°C$ in a thermostatic bath.

The relative viscosity of each solution is determined by the following empirical formula:

$$\eta_\rho = \frac{ds \times ts}{dw \times tw}$$

The values of viscosities (η) and relative viscosities (η_r) of various systems in different percentages of dioxane-water and methanol-water mixtures are represented in Tables 1–6.

The relative viscosities have been analyzed by the Jones-Dole equation

$$\frac{\eta_r - 1}{\sqrt{c}} = A + B\sqrt{c}$$

where C = molar concentration of the ligand solution, A = viscosity coefficient

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which measures solute-solute interaction and B = viscosity coefficient which measures the interaction between solvent solute.

Graphs are plotted between $\frac{\eta_{r-1}}{\sqrt{c}}$ *vs.* $\sqrt{c}$. The graph for each system gives a straight line showing the validity of Jones-Dole equation. The slope of the straight line gives the value of β-coefficient.

TABLE-1
VISCOSITY OF L_1 IN DIFFERENT PERCENTAGES OF DIOXANE-WATER

Dioxane (%)	Density (g/cc)	T_s (s)	C (mol/L)	η_r	η_{sp} (cp)	$\eta_r - 1/c$
70	1.1423	164	0.010	1.2514	0.2584	2.3884
75	1.1594	184	0.015	1.4157	0.4197	0.4117
80	1.1771	196	0.020	1.5219	0.5119	3.6196
85	1.1895	204	0.025	1.6056	0.6056	3.8301

TABLE-2
VISCOSITY OF L_2 IN DIFFERENT PERCENTAGES OF DIOXANE-WATER

Dioxane (%)	Density (g/cc)	T_s (s)	C (mol/L)	η_r	η_{sp} (cp)	$\eta_r - 1/c$
70	1.1425	150	0.010	1.0070	0.0070	0.0700
75	1.1596	167	0.015	1.0091	0.0091	0.0074
80	1.1780	184	0.020	1.0113	0.0113	0.0074
85	1.1897	204	0.025	1.0168	0.0168	0.1062

TABLE-3
VISCOSITY OF L_3 IN DIFFERENT PERCENTAGE OF DIOXANE-WATER

Dioxane (%)	Density (g/cc)	T_s (s)	C (mol/L)	η_r	η_{sp} (cp)	$\eta_r - 1/c$
70	1.1427	155	0.010	1.0084	0.0084	0.084
75	1.1596	192	0.015	1.0107	0.0107	0.087
80	1.1780	196	0.020	1.0129	0.0129	0.091
85	1.1897	212	0.025	1.0150	0.0150	0.094

TABLE-4
VISCOSITY OF L_1 IN DIFFERENT PERCENTAGES OF METHANOL-WATER

Dioxane (%)	Density (g/cc)	T_s (s)	C (mol/L)	η_r	η_{sp} (cp)	$\eta_r - 1/c$
70	1.0317	258	0.010	0.7011	0.7010	7.011
75	1.0299	232	0.015	0.5617	0.5617	4.586
80	1.0256	204	0.020	1.3415	0.3415	2.414
85	1.0223	298	0.025	1.3148	0.3146	1.989

TABLE-5

VISCOSITY OF L_2 IN DIFFERENT PERCENTAGE OF METHANOL-WATER

Dioxane (%)	Density (g/cc)	T_s (s)	C (mol/L)	η_r	η_{sp} (cp)	$\eta_r - 1/c$
70	1.0319	244	0.010	1.6179	0.6179	6.179
75	1.0290	226	0.015	1.2303	0.2303	1.880
80	1.0256	199	0.020	1.0561	0.0561	0.357
85	1.0223	176	0.025	1.0112	0.0112	0.078

TABLE-6

VISCOSITY OF L_3 IN DIFFERENT PERCENTAGE OF METHANOL-WATER

Dioxane (%)	Density (g/cc)	T_s (s)	C (mol/L)	η_r	η_{sp} (cp)	$\eta_r - 1/c$
70	1.0320	232	0.010	1.2640	1.2640	2.640
75	1.0297	214	0.015	1.0786	1.0786	0.642
80	1.0258	176	0.020	1.0224	1.0224	0.158
85	1.0226	125	0.025	1.0.112	1.0112	0.071

It is observed from Table-7 that β-coefficient value of ligand L_1 is very high as compared to the ligand L_2 and L_3 systems in different percentages of dioxane. It shows that there is stronger interaction between solvent and solute ligand molecule for ligand L_1 system and weaker interaction between solvent and solute for ligand L_2 and L_3 systems. This may be due to chloro-bromo and chloro-nitro stronger electron withdrawing groups which may strongly affect the value of β-coefficient.

TABLE-7

LIGAND MIXTURE β-COEFFICIENT VALUE

Ligand	Mixture	β-Cofficient value $(L\ mol^{-1})$
Ligand 1 (L_1)	Dioxane-water	29.500
Ligand 2 (L_2)	Dioxane-water	0.025
Ligand 3 (L_3)	Dioxane-water	2.000
Ligand 1 (L_1)	Methanol-water	−1.000
Ligand 2 (L_2)	Methanol-water	−1.770
Ligand 3 (L_3)	Methanol-water	−20.000

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