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STUDY OF MOLECULAR INTERACTIONS IN TERMS OF VISCOSITY, β-COEFFICIENT OF DIFFERENT LIGANDS IN DIFFERENT CONCENTRATIONS OF ORGANIC SOLVENT-WATER MIXTURES IN DIFFERENT CONCENTRATIONS

J B Devhade[*1], K N Sonune[2], M J Devade[3] and S S Kalwaghe[4]
Department of Chemistry, Jijamata Mahavidyalaya, Buldana – 443001 (M.S.) India[*1,2,3,4]

ABSTRACT

The study of molecular interactions in terms of viscosity, β-coefficient of different ligands in different concentrations of Acetone-water and Ethanol-water mixtures in different concentrations is undertaken. Relative viscosity of ligand solutions decreases with increase in the concentration of ligand may be attributed to increase in solute - solvent interactions. The β-coefficient is an adjustable parameter, which may be either positive or negative and it is a measure of the effective hydrodynamic volume of solute which accounts for the solute - solvent interactions

Keywords: viscosity, β-coefficient, solute – solvent interaction.

I. INTRODUCTION

Various researcher's are interested to find out binary liquid mixture interactions along with solute. Viscosity is developed in liquids because of shearing effect of moving one layer of liquid past another motion of liquid can be visualized as a movement of one layer over another . A layer in contact with stationary surface remains stationary. The second layer move slowly, third move quickly then second and so on. This type of flow is called laminar flow or streamlined flow.

Viscosities are measured by different methods. In the Ostwald viscometer, the time taken for the solution to flow through the capillary is noted. Care was taken to ensure that the temperature is both constant and uniform. The method is very suitable for determining γ, because the ratio of the viscosities of the solution and the pure solvent is proportional to the drainage time 't'. Here the principle of the Ostwald viscometer routinely used for measurements on liquids and solutions, in which capillary flow is induced by gravity. The time of flow is proportional to the viscosity divided by the liquid density.

Useful information about solute-solute and solute -solvent interaction provides when the behaviour of electrolytes are studied by viscometry . Many workers [1-3] have been studied these interactions in aqueous and non -aqueous solutions. Ikhe[4] has studied the viscosity of [HBMPPI] ,[AHBMPPP] , [PHNMPMPP] and captopril in 70% dioxane water mixture at different concentrations. Molecular interactions of electrolyte in binary mixture of two liquids in terms of viscosity , β - coefficient have been studied by Metrotra and many workers [5-8].

Recently, Raghuwanshi et al[9] studied solute - solvent interaction at different concentration and different percentage of solvent for substituted pyrazolines. Tambatkar G.D.[10] have studied viscosity and β - coefficient value of some heterocyclic and non-heterocyclic drugs in 70 % Dioxane-water mixture solution.

The present study deals with the study of molecular interactions in terms of viscosity, β-coefficient of different ligands in different concentrations of Acetone-water and Ethanol-water mixtures in different concentrations.

II. EXPERIMENTAL

The viscosities were measured by means of Ostwald's Viscometer $(\pm 0.11\% Kgm^{-1}s^{-1})$ which was kept in equilibrium with elite thermostatic water bath (± 0.1 °C) . Ligand solutions of different concentrations were prepared in 70 % Acetone-water and ethanol - water.

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

$$\eta_r = (ds \times ts) / (dw \times tw) \qquad \text{--(1)}$$

Where η_r = relative viscosity of ligand solution,

ds = density of ligand solution ,

dw=density of distilled water,
ts=time of flow for solution,
tw=time of flow for distilled water

The relative viscosity and density data for ternary mixture at different concentrations are presented in Tables 1 to 6

The relative viscosities have been analysed by Jones -Dole equation

$$(\eta_r - 1) / \sqrt{c} = A + B \sqrt{c} \text{--(2)}$$

Where   C =molar concentration of the ligand solution ,
A=Falkenhagen coefficient,
B=Jones-Dole coefficient

A is the measure of solute - solute interactions and B is the measure of solute - solvent interaction .

The graphs are plotted between $(\eta_r - 1) / \sqrt{c}$ Vs. $\sqrt{c}$. The graph for each system gives linear straight line showing validity of Jones - Dole equation. The slope of straight line gives value of β- coefficient.

In the present study, relative viscosity of ligand solutions decreases with increase in the concentration of ligand may be attributed to increase in solute - solvent interactions.

From the graph of $(\eta_r - 1) / \sqrt{c}$ versus $\sqrt{c}$, `A' which is the measure of solute - solute interactions and `B' which is the measure of solute - solvent interactions has been calculated .

Table -1
Densities and viscosities of systems in Acetone at 25ºC(±0.1ºC) System: Ligand -L₁(Allopurinol)

Sr. No.	Concentration C (mole/liter)	$\sqrt{c}$ x10^{-2} (mole$^{1/2}$/liter$^{1/2}$)	Density (gm./c.c.)	Time (sec.)	η_r	η_r-1/$\sqrt{c}$
1	60 x 10^{-4}	7.7460	0.871	50	1.1496	1.9303
2	70 x 10^{-4}	8.3666	0.848	43	0.9626	-0.4468
3	80 x 10^{-4}	8.9443	0.830	35	0.7672	-2.6040
4	90 x 10^{-4}	9.4868	0.807	28	0.5967	-4.2487
5	100 x 10^{-4}	10.0000	0.784	22	0.4555	-5.445

Table -2
Densities and viscosities of systems in Acetone at 25ºC(±0.1ºC) System: Ligand -L₂(Acenocoumarol)

Sr. No.	Concentration C (mole/liter)	$\sqrt{c}$ x10^{-2} (mole$^{1/2}$/liter$^{1/2}$)	Density (gm./c.c.)	Time (sec.)	η_r	η_r-1/$\sqrt{c}$
1	60 x 10^{-4}	7.7460	0.871	51	1.1726	2.2271
2	70 x 10^{-4}	8.3666	0.848	46	1.0297	0.3548
3	80 x 10^{-4}	8.9443	0.831	37	0.8116	-2.074
4	90 x 10^{-4}	9.4868	0.807	29	0.6178	-4.0274
5	100 x 10^{-4}	10.0000	0.785	22	0.4559	-5.4410

Table -3
Densities and viscosities of systems in Acetone at 25ºC(±0.1ºC) System: Ligand-L₃(Warfarin)

Sr. No.	Concentration C (mole/liter)	$\sqrt{c}$ x10^{-2} (mole$^{1/2}$/liter$^{1/2}$)	Density (gm./c.c.)	Time (sec.)	η_r	η_r-1/$\sqrt{c}$
1	60 x 10^{-4}	7.7460	0.871	52	1.1961	2.5303
2	70 x 10^{-4}	8.3666	0.848	46	1.0301	0.3596
3	80 x 10^{-4}	8.9443	0.831	37	0.8120	-2.1029
4	90 x 10^{-4}	9.4868	0.807	28	0.5967	-4.2497
5	100 x 10^{-4}	10.0000	0.785	23	0.4768	-5.2320

Table -4
Densities and viscosities of systems in Ethanol at 25ºC(±0.1ºC) System: Ligand -L_1 (Allopurinol)

Sr. No.	Concentration C (mole/liter)	$\sqrt{c}$ x10^{-2} (mole$^{1/2}$/liter$^{1/2}$)	Density (gm./c.c.)	Time (sec.)	η_r	η_r-1/$\sqrt{c}$
1	60 x 10^{-4}	7.7460	0.854	97	2.1309	14.5922
2	70 x 10^{-4}	8.3666	0.827	95	2.0210	14.4564
3	80 x 10^{-4}	8.9443	0.809	87	1.8105	9.0660
4	90 x 10^{-4}	9.4868	0.796	73	1.4947	5.2129
5	100 x 10^{-4}	10.0000	0.785	59	1.1914	1.9140

Table -5
Densities and viscosities of systems in Ethanol at 25ºC(±0.1ºC) System: Ligand -L_2 (Acenocoumarol)

Sr. No.	Concentration C (mole/liter)	$\sqrt{c}$ x10^{-2} (mole$^{1/2}$/liter$^{1/2}$)	Density (gm./c.c.)	Time (sec.)	η_r	η_r-1/$\sqrt{c}$
1	60 x 10^{-4}	7.7460	0.856	96	2.1136	14.3690
2	70 x 10^{-4}	8.3666	0.829	93	1.9830	11.7443
3	80 x 10^{-4}	8.9443	0.812	89	1.8588	9.6063
4	90 x 10^{-4}	9.4868	0.801	74	1.5246	5.5279
5	100 x 10^{-4}	10.0000	0.787	58	1.1741	1.7410

Table -6
Densities and viscosities of systems in Ethanol at 25ºC(±0.1ºC) System: Ligand -L_3 (Warfarin)

Sr. No.	Concentration C (mole/liter)	$\sqrt{c}$ x10^{-2} (mole$^{1/2}$/liter$^{1/2}$)	Density (gm./c.c.)	Time (sec.)	η_r	η_r-1/$\sqrt{c}$
1	60 x 10^{-4}	7.7460	0.855	97	2.1334	14.6245
2	70 x 10^{-4}	8.3666	0.829	94	2.0045	12.0012
3	80 x 10^{-4}	8.9443	0.812	89	1.8590	9.6085
4	90 x 10^{-4}	9.4868	0.800	73	1.5022	5.2919
5	100 x 10^{-4}	10.0000	0.786	58	1.1727	1.7270

III. RESULT & DISCUSSION

The large and small values of `A' show the stranger and weaker solute - solute interactions respectively as listed in following tables 7-8 .

Table-7

A and B coefficient values in Acetone Medium

Sr. No.	System	A	B(lit/mole)
1	Lgand-1	27.30	-3.307
2	Lgand-2	29.44	-3.505
3	Lgand-3	30.21	-3.586

Table-8
A and B coefficient values in Ethanol Medium

Sr. No.	System	A	B(lit/mole)
1	Lgand-1	63.47	-6.109
2	Lgand-2	58.13	-5.560
3	Lgand-3	59.83	-5.745

When the solute is introduced into solvent of organic - water mixture, it will interfere with the ordered structure of water in the solute's cosphere. It is evident from Table No.7 to Table No. 8, that the β-coefficient is an adjustable parameter, which may be either positive or negative and it is a measure of the effective hydrodynamic volume of solute which accounts for the solute - solvent interactions. It is known as a measure of order or disorder introduced by the solute into the solvent.

Solutes with positive viscosity β-coefficient are characterized as "Structure formers" and will impose a new order by reorientation of the adjacent water molecules indicating strong solute- solvent interactions. Solutes with negative viscosity β- coefficient is characterized as "Structure Breakers" indicating weak solute - solvent interactions.

Physical properties of liquids, binary liquids and ternary liquids have been subject of interest of research laboratory[11-13]. The change structure of solvent or solution as a result of hydrogen bond formation or breaking leads to decrease or increase in interaction. Hydrophobic (structure making) or hydrophilic (structure breaking) character of solute , i. e. hydrogen bond formation or breaking properties can be correlated with changes in density or viscosity . Solute can occupy the interstial space in solvent

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