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"THERMODYNAMIC STUDY OF SUBSTITUTED THIOCARBAMIDO-NAPHTHOLS AT DIFFERENT CONCENTRATIONS AND DIFFERENT TEMPERATURES IN MIXED SOLVENT MEDIA"

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ABSTRACT

Conductivity play vital role in drug diffusion. Thermodynamic parameters affected by substituent's of drug. Thus recently in laboratory, conductometrically have been investigated thermodynamic parameters of 5-Phenylthiocarbamido-1-naphthol [PTCN] or L_2 and 5-p-Tolyl -thiocarbamido-1-naphthol [p-MPTCN] or L_4 have been studied at different concentrations in 80% ethanol-water mixture at different temperatures. This work highlights investigation of G, K and μ values. The thermodynamic parameters viz. ΔH, ΔS and ΔG for ion pair formation determine from the value of ion association constant at 298K and 303K. This investigation provided valuable information regarding to solute-solvents, solute–solute and solvent-solvent interaction, effect of various substituent's of drugs and effect of dilution from conductometric measurements of 5-Phenyl -thiocarbamido-1-nahthol and 5-p-Tolylthiocarbamido-1-naphthol.

KEYWORDS: Thermodynamic parameters, 5-Phenylthiocarbamido-1-nahthol [PTCN] and 5-p-Tolylthiocarbamido-1-naphthol or L_4 [p-MPTCN].

INTRODUCTION

Conductrometric measurments of electrolytic solution provided valuable information concerned to solubility and permeability of drugs, which are essential biopharmaceutical parameters. These two parameters are accountable for effective bioavailability and good in vitro and vivo correlation.[1] Now-a-days pharmaceutical technologist has great challenge to enhance solubility and dissociation rate and oral bioavailability of weakly water soluble drugs.[2] Hydrotropic solubalisation is considered as one of the sophisticated methods of solubalisation.[3] Enhance aqueous solubalisation of insoluble drugs by adding hydrotropic agents. Number of researchers work on effect of solubility enhancers[4-5] and due to that increase solubility of drugs but no detail explanation available regarding to these improving solubility. `The split of electrolyte conductivities into the ionic components ideally requires transference numbers, the accurate measurements of which present serious experimental problems in many non-aqueous solvents. Conductometric measurments provided valuable information about solute-solute and solute-solvent interaction [6]. Many researchers studied conductometric measurements of electrolytic solution in aqueous and non aqueous solutions Conductance measurements and drugs activity correlation provide valuable information concerned with investigation of drug-receptor interactions, transport property of drugs and ion-solvent interactions.[7-18] Conductrometrically investigation of ionic association of divalent asymmetric electrolyte $Cu(NO_3)_2$ with Kryptofix-22 in mixed (CH_3OH-DMF) solvents at different temperatures was carried out by Gomma and Al-Jahdalli.[19] Present work concern to effect of different substituent's on conductometric properties, thermodynamic behavior and Walden product of 5-Phenylthiocarbamido-1-naphthol and 5-p-Tolylthiocarbamido-1-naphthol at different concentrations and at 298K and 303K. Shedlovsky method[20] used for data analysis. Recently observed values of association constant at various concentrations which help to examine thermodynamic parameters like ΔH; ΔS and ΔG

MATERIALS AND METHOD

All reagents and chemicals were procured from commercial sources (SD Fine Chemicals, India; Aldrich, USA) and used without any further purification. In present investigation used all freshly prepared solution. To Prepared 0.01M, 0.005M. 0.0025 M and 0.0012 M solutions of 5-Phenylthiocarbamido-1-naphthol and 5-p-Tolylthiocarbamido-1-naphthol. Maintain thermal equilibrium (298K and 303K) of drugs solution by using thermostat. After getting thermal equilibrium, conductivity of those electrolyte solutions was measured.

RESULT AND DISCUSSION

Prepared 0.01, 0.005 M, 0.0025M and 0.0012 M solutions of L_2 and L_4 in 80% ethanol-water mixture respectively. To measured conductance of each solutions by using conductivity bridge at 298K and 303K respectively. Resultant data tabulated in **Table-1 to Table-2**

.

Table 1: Conductometric Measurements At Different Concentrations Of 5-Phenylthiocarbamido-1-Naphthol[L_2]

Determination OF G, K And μ At 80% Ethanol-Water Mixture				
Temp.	**Concentration C (M)**	**Observed conductance (G)**	**Specific conductance (k)**	**Molar conductance (μ)**
298k	0.01	0.03062	0.003572 X 10^{-3}	0.357233
	0.005	0.01568	0.001887 X 10^{-3}	0.377548
	0.0025	0.0107	0.001362 X 10^{-3}	0.545015
	0.0012	0.00828	0.001059 X 10^{-3}	0.882578
303k	0.01	0.0309	0.003684 X 10^{-3}	0.368487
	0.005	0.01656	0.002055 X 10^{-3}	0.411067
	0.0025	0.01119	0.001421 X 10^{-3}	0.568588
	0.0012	0.00904	0.001145 X 10^{-3}	0.954592

Table 2: Conductometric Measurements At Different Concentrations Of 5-P-Tolyl - thiocarbamido-1-Naphthol [L_4]

Determination OF G, K And μ AT 80% Ethanol-Water Mixture				
Temp.	**Concentration C (M)**	**Observed conductance (G)**	**Specific conductance (k)**	**Molar conductance (μ)**
298K	0.01	0.02082	0.002429 X 10^{-3}	0.2429
	0.005	0.0134	0.001613 X 10^{-3}	0.32264977
	0.0025	0.0087	0.001107 X 10^{-3}	0.443142857
	0.0012	0.00862	0.001102 X 10^{-3}	0.918819358
303K	0.01	0.02161	0.002577 X 10^{-3}	0.257702139
	0.005	0.01262	0.001566 X 10^{-3}	0.313264457
	0.0025	0.00966	0.001227 X 10^{-3}	0.490845091
	0.0012	0.0952	0.001206 X 10^{-3}	1.05277778

Determine the specific constant (Ksp), log (Ksp) and thermodynamic parameters viz. change in free energy (ΔG), change in entropy (ΔS) and change in enthalpy (ΔH) of [p-MPTCN] at various molar concentration and at same temperature by known literature methods. The results obtained were given in **Table-3 and 4.**

Table-3 : Conductometrically Determination Of Ksp, Log Ksp, ΔG, ΔH And ΔS At Different Concentration And Different Temperatures In 80% Ethanol-Water Mixture

System: 5-Phenylthiocarbamido-1-Naphthol L_2-[PTCN]						
Temp	**Conc. C (M)**	**Ksp 10^{-3}**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
298 K	0.01	0.00549	-4.26015	24307.79	-76850.9	-339.459
	0.005	0.0153	-4.81417	27468.94	-86846.1	-383.607
	0.0025	0.007995	-5.09736	29084.77	-91954	-406.17
	0.0012	0.004836	-5.31619	30333.37	-95902.2	-423.609
303K	0.01	0.0970	-4.30373	24968.44	-80244.5	-347.237
	0.005	0.0155	-4.81081	27910.3	-89699	-388.15
	0.0025	0.00739	-5.1311	29768.49	-95671.5	-413.993
	0.0012	0.00486	-5.31857	30856.15	-99166.7	-429.118

Table-4 : Conductometrically Determination Of Ksp, Log Ksp, ΔG, ΔH And ΔS At Different Concentration And Different Temperatures In 80% Ethanol-Water Mixture						
System: 5-P-Tolylthiocarbamido-1-Naphthol L_4-[p-MPTCN]						
Temp	**Conc. C (M)**	**Ksp 10^{-3}**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
298K	0.01	0.02539	-4.5952	26219.53	-82895.5	-366.158
	0.005	0.01120	-4.95066	28247.69	-89306.3	-394.476
	0.0025	0.005283	-5.27709	30110.28	-95197.2	-420.495
	0.0012	0.005233	-5.28124	30133.93	-95310.1	-420.953
303K	0.01	0.02430	-4.61434	26770.45	-86036.6	-372.3
	0.005	0.008978	-5.04681	29279.49	-94100.1	-407.193
	0.0025	0.005510	-5.2588	30509.38	-98052.4	-424.296
	0.0012	0.005322	-3.27364	18992.28	-60999.5	-263.999

CONCLUSION

Table-1 and 2 showed that observed conductance (G), specific conductance (k) decreases while molar conductance (μ) were increases continuously along with decreasing molar concentrations from 0.01M to 0.0012M. G, k and μ increases along with rising temperatures for both ligands (L_2 and L_4). **Table-3 and 4** revel that values of Ksp, log Ksp , ΔH and ΔS decreases continuously while ΔG increases along with decreasing molar concentration from 0.01M to 0.0012M and rising temperatures respectively for both ligands (L_2 and L_4). From **Table- 1 and 2** it concludes that L_2 has more values of conductance than L_4. Because L_2 has phenyl substituent, it stabilized structure while this was not happen in Tolyl group cause of +I effect of -CH3 group. These parameters directly influence by structure as well as nature of drugs. The change in thermodynamic parameters values closely affected by molar concentrations and temperatures. These parameters shackle by another factors viz. the solute (drug)-solvent interactions, solvent-solvent interactions, solvent-solvent-solute interactions and solute-solute-solvent interactions. This type investigation supporting to pharmacodynamics and pharmacokinetics study of drugs.

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