Conductometric Study of Substitutedthiocarbamidonaphthols in 70% Ethanol–Water Mixture at Different Molar Concentrations at Constant Temperature

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Abstract: ***Recently in this laboratory conductrometric investigation of 5-phenylthiocarbamido-1-naphthol, 5-p-chlorophenylthiocarbamido-1-naphthol and 5-p-tolylthiocarbamido-1-naphthol, have been carried out at different concentrations of solute in 70% ethanol-water mixture at constant temperature. G, K and µ values are determined. The thermodynamic parameters viz. ΔH, ΔS and ΔG for the ion pair formation determine from the value of ion association constant at constant temperature. 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 the present conductometric measurements.***

Keywords: Thermodynamic parameters, 5-phenylthiocarbamido-1-naphthol [PTCN], 5-p-chlorophenylthiocarbamido-1-naphthol [p-CPTCN] and 5-p-tolylthiocarbamido-1-naphthol [p-MPTCN].

1. Introduction

Number of ions of electrolyte in solution decide the conduction of electrolytic solution. Conductrometric measurements 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 the solubility and dissociation rate and oral bioavailability of weakly water soluble drugs[2]. Hydrot ropic solubalisation is considered as one of the sophisticated methods of solubalisation[3] Enhance the aqueous solubalisation of insoluble drugs by adding hydrotropic agents. Number of researchers work on the 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]. Conductrometrically investigation of the ionic association of divalent asymmetric electrolyte $Cu(NO_3)_2$ with Kryptofix-22 in mixed (MeOH-DMF) solvents at different temperatures was carried out by Gomma and Al-Jahdalli[7]. Many researchers were studied the alkali metal at different proportion of mixed solvents by conductometrically[8]-[9]. Very few researchers investigated the thermodynamic parameter and Walden product of different complexes and they also examine the comparison of transition metal complexes among the halide group[10]-[14]. Singh et al[15] was investigated the ion pair formation and thermodynamic parameters of Glycine Bis-1-amidino-O-methylurea Co(III) halides in water-methanol mixture at different temperatures[15]. Conductometric study of nimesulide in aqueous solutions of hydrotropic agents at different temperatures was carried out by solanki et al[16].

Present work concern to investigation of conductometric properties, thermodynamic behavior and Walden product of 5-phenylthiocarbamido-1-naphthol, 5-p-chlorophenylthio-carbamido-1-naphthol and 5-p-tolylthiocarbamido-1-naphthol in 70% ethanol-water mixture at different concentration and at constant temperature i.e. 298K. Shedlovsky method[17] used for the data analysis. Recently observed values of association constant at various concentrations which help to examine the thermodynamic parameters like ΔH, ΔS and ΔG for the formation. Resultant values help to examine the nature of different interactions.

2. Experimental

In present investigation used all the freshly prepared solution. All the chemicals and solvents used for the synthesis were of A.R. grade. The solvents were purified by standard method. Prepared different concentration solutions of 5-phenylthiocarbamido-1-naphthol, 5-p-chlorophenylthio caraamido-1-naphthol and 5-p-tolylthiocarb amido-1-naphthol viz. 0.01M, 0.005M. 0.0025M and 0.0012M by using 70% ethanol-water mixture. Maintain the thermal equilibrium (298K) of drugs solution by using thermostat. After getting thermal equilibrium, conductivity of that electrolyte was measured.

3. Result and Discussion

Firstly prepared the solution of 0.01 M concentration then by the serial dilution method prepared the solutions of 0.005M,

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0.0025M and 0.0012M with 70% ethanol-water mixture. Measured the conductance of the each solution by using conductivity bridge at 298K. Result obtained are given in **Table-1 to Table-6.** From the data observed conductance (G), specific conductance (k) and molar conductance (μ) were determined by known literature method.

Table 1: Conductometric Measurements At Different Concentration Of [PTCN]

DETERMINATION OF G, k and μ AT DIFFERENT CONCENTRATIONS At 298 K				
% of Ethanol-Water-	Conc. C (M)	Observed conductance (G)	Specific conductance (k)	Molar conductance (μ)
70%	0.01	0.02381	0.002777×10^{-3}	0.277783
	0.005	0.01492	0.001796×10^{-3}	0.359249
	0.0025	0.00965	0.001228×10^{-3}	0.491532
	0.0012	0.00812	0.001036×10^{-3}	0.865524

Table 2: Conductometric Measurements At Different Concentration of [p-CPTCN]

DETERMINATION OF G, k and μ AT DIFFERENT CONCENTRATIONS At 298 K				
% of (Ethanol-Water)	Conc. C (M)	Observed conductance (G)	Specific conductance (k)	Molar conductance (μ)
70%	0.01	0.01493	0.001741×10^{-3}	0.1741833
	0.005	0.01145	0.001378×10^{-3}	0.275697
	0.0025	0.01044	0.001329×10^{-3}	0.5317714
	0.0012	0.00982	0.001256×10^{-3}	1.0467292

Table 3: Conductometric Measurements At Different Concentration of [p-MPTCN]

DETERMINATION OF G, k and μ AT DIFFERENT CONCENTRATIONS At 298 K				
% of (Ethanol-Water)	Conc. C (M)	Observed conductance (G)	Specific conductance (k)	Molar conductance (μ)
70%	0.01	0.01783	0.00208×10^{-3}	0.208017
	0.005	0.01139	0.00137×10^{-3}	0.274252
	0.0025	0.00865	0.00110×10^{-3}	0.440596
	0.0012	0.00753	0.00096×10^{-3}	0.802635

Table-1, 2 and 3 showed that the observed conductance (G), specific conductance (k) decreases while molar conductance (μ) were increases continuously. The specific conductance decreases and molar conductance increases along with decreasing molar concentrations. The above parameters values are higher in case of [PTCN] than [p-CPTCN] and [p-MPTCN]. In case of [p-CPTCN] and [p-MPTCN] phenyl ring substituted by –Cl and $–CH_3$ group respectively which are electrons releasing group while in case of [PTCN] phenyl ring free.

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-4, 5 and 6.**

Table 4: Conductometric Measurements at Different Concentration of Drug [PTCN]

DETERMINATION OF Ksp, log Ksp, ΔG,ΔH and ΔS AT DIFFERENT CONCENTRATIONS AND AT 298 K					
SYSTEM: [PTCN]			Medium - 70% ETHANOL-Water		
Conc. C (M)	Ksp	Log Ksp	ΔG	ΔH	ΔS
0.01	0.00332	-4.4786	25554.47	-80793.6	-356.87
0.005	0.00139	-4.8573	27715.17	-87624.1	-387.04
0.0025	0.00654	-5.187	29596.66	-93572.9	-413.32
0.0012	0.00464	-5.3331	30430.08	-96207.3	-424.96

Table 5: Conductometric Measurements At Different Concentration Of Drug [p-CPTCN]

DETERMINATION OF Ksp, log Ksp, ΔG,ΔH and ΔS AT DIFFERENT CONCENTRATIONS AND AT 298 K					
SYSTEM: [p-CPTCN]			Medium - 70% ETHANOL-Water		
Conc. C (M)	Ksp	Log Ksp	ΔG	ΔH	ΔS
0.01	0.0131	-4.88404	27867.62	-88108.3	-389.181
0.005	0.0081	-5.08725	29027.1	-91774.2	-405.374
0.0025	0.0076	-5.11873	29206.69	-92341.4	-407.879
0.0012	0.0067	-5.16803	29487.98	-93229	-411.802

Table 6: Conductometric Measurements At Different Concentration Of Drug [p-MPTCN]

DETERMINATION OF Ksp, log Ksp, ΔG,ΔH and ΔS AT DIFFERENT CONCENTRATIONS AND AT 298 K					
SYSTEM: [p-MPTCN]			**Medium - 70% ETHANOL-Water**		
Conc. C (M)	*Ksp*	*Log Ksp*	*ΔG*	*ΔH*	*ΔS*
0.01	0.0186	-4.72986	26987.87	-85325.3	-376.89
0.005	0.008	-5.09182	29053.14	-91855.6	-405.734
0.0025	0.0052	-5.2821	30138.84	-95286.1	-420.889
0.0012	0.0039	-5.39866	30803.93	-97390.1	-430.181

Table-4, 5 and 6 revel that when we moving from molar concentration 0.01M to 0.0012M concentration solutions the value of Ksp , log Ksp , ΔH and ΔS decreases continuously while ΔG increases. These parameters directly influence by the structure as well as nature of drugs. The change in thermodynamic parameters values closely affected by the temperature, molar concentrations and percentage compositions. Thermodynamic parameters are directly hampered by other aspect such as solute (drug)-solvent interactions, solvent-solvent interactions, solvent-solvent-solute interactions and solute-solute-solvent interactions. Internal geometry of drugs and internal or intra hydrogen bonding are also interfere in these parameters. In this investigation it is found that molar conductance of [PTCN] is comparatively higher than [p-CPTCN] and [p-MPTCN]. From this observation it is conclude that [PTCN] has more drug effect than [p-CPTCN] and [p-MPTCN].

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ISSN (Online): 2319-7064
Index Copernicus Value (2013): 6.14 | Impact Factor (2014): 5.611

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