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Determination of ΔH, ΔS and ΔG of [MDA] and [EDA] by Conductometric Studies

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ABSTRACT

Conductivity play vital role in molecule; diffusion, transmission, metabolisum (molecule activity and molecule effect) and exerition in pharmokinetics and pharmodynamics of molecules. Thermodynamic parameters affected by substituent's of molecule. Considering these facts recently in this laboratory, conductometrically thermodynamic parameters of 5-(1-methylamino-2,4-dithiobiureto)aminoindole [MDA] and 5-(1-ethylamino-2,4-dithiobiureto)aminoindole [EDA] were investigated at different molar concentrations and different percentage compositions. This work mainly highlights on investigation of G, K and μ values. The thermodynamic parameters viz. ΔH, ΔS and ΔG for ion pair formation were determined from the value of ion association constant at 303.15 K This technique is suitable and accurate to study pharmokinetics and pharmodynamics parameters.

Keywords: Conductometric measurements, thermodynamic parameters, [MDA], [EDA]

I. INTRODUCTION

Organic chemistry of 2,4-dithiobiureto nuclei contain heterocycles and heteroacycles revealed distinct effects of these compounds are due to their strong biological activities[1–12]. Indoles showed antimicrobial, anti-inflammatory, anti-cancer and anti-oxidant activities[13-15]. These 2,4-dithiobiurets can also be used as intermediates for synthesis of numerous heterocycles with notable biological activities[16–19]. The biological uses of 2,4-dithiobiuret are altered by different substitutions on its nitrogen atom. Numerous 2,4-dithiobiurests were produced as part of a larger lab program to manufacture heteroacycles, and these were then converted into 5, 6, and 7 member heterocycles[20].

With conductometric measurements G, K and μ values, ΔH, ΔS and ΔG can be determined and which provided theoretical information about medicine/molecule activity[21].

Conductance measurements provide very important and valuable information regarding ion-ion and ion-solvent interactions[22,23]. Conductance of alkali metal in different mixtures mixed solvents were reported[24,25]. The

thermodynamic parameters and Walden products of different complexes were studied by few researcher and they also determined the comparison of transition metal complexes among the halide groups[26]. Interaction between sodium sulphate and 1-propanol, 1-butanol, 1-pentanol and 1-hexanol at different temperatures were determined by conductometric technique[27].

The present study deals with an investigation of conductometric properties, thermodynamic behaviour and Walden product of 5-(1-methylamino-2,4-dithiobiureto)aminoindole [MDA] and 5-(1-ethylamino-2,4-dithiobiureto)aminoindole [EDA] in ethanol-water mixture at different concentrations and different percentage compositions at constant temperature 303.15 K.

II. EXPERIMENTAL

All the chemicals and solvents used for the synthesis were of A.R. grade. All the freshly prepared solutions were used for investigations. Different concentration solutions of 0.1M of 5-(1-methylamino-2,4-dithiobiureto)aminoindole [MDA] and 5-(1-ethylamino-2,4-dithiobiureto)aminoindole [EDA] were prepared. 0.1M solution of [MDA] and [EDA] was prepared and then by serial dilution method, 0.075 M, 0.050 M and 0.025 M were prepared in 100% water and ethanol-water mixture respectively. Similar solutions were prepared for 80% and 70% water-ethanol mixture. All the solutions of molecule were always used a fresh in the present investigation.

In 50 ml glass beaker [MDA] solution was taken and it was kept inside the thermostat for 15-20 minutes to attain the thermal equilibrium 303.15 K. After achieving the thermal equilibrium, the conductivity was measured. Similar procedure was adopted for [EDA].

III.RESULTS AND DISCUSSION:

During this investigation conductometric measurements of 100%, 80%, and 70% mixtures of water-ethanol were prepared. In first set 0.1M solution of [MDA] and in second set 0.1M solution of [EDA] was prepared in conductivity water and by serial dilution method 0.075M, 0.050M and 0.025M solutions were prepared. At 303.15 K the conductance of each solution was measured by conductivity bridge and result are cited in **Table 1** and **Table 2**. From the data observed conductance (G), specific conductance (k) and molar conductance (μ) were determined by known literature method.

Table 1: Conductometric Measurements of [MDA] at different concentration

Determination of G, k and μ on different Concentrations at 303.15 K

% of solution (**Water-ethanol**)	Concentration (M)	Observed conductance (G)	Specific conductance (k)	Molar conductance (μ)
100%	0.1 M	0.58 X 10^{-3}	0.550961 X 10^{-3}	5.689606
	0.075 M	0.49 X 10^{-3}	0.465317 X 10^{-3}	6.450887
	0.050 M	0.35 X 10^{-3}	0.332092 X 10^{-3}	7.021847
	0.025 M	0.19 X 10^{-3}	0.179836 X 10^{-3}	7.973448
80%	0.1 M	0.71 X 10^{-3}	0.674669 X 10^{-3}	6.926687
	0.075 M	0.68 X 10^{-3}	0.646121 X 10^{-3}	8.861609

	0.050 M	0.59 X 10^{-3}	0.560477 X 10^{-3}	11.58953
	0.025 M	0.39 X 10^{-3}	0.370156 X 10^{-3}	15.58626
70%	0.1 M	0.23 X 10^{-3}	0.2179 X 10^{-3}	2.359003
	0.075 M	0.2 X 10^{-3}	0.189352 X 10^{-3}	2.771363
	0.050 M	0.18 X 10^{-3}	0.17032 X 10^{-3}	3.786404
	0.025 M	0.12 X 10^{-3}	0.113224 X 10^{-3}	5.308966

Table 2: Conductometric Measurements of [EDA] at different concentration

Determination of G, k and μ on different Concentrations at 303.15 K

% of solution (**Water-ethanol**)	Concentration (M)	Observed conductance (G)	Specific conductance (k)	Molar conductance (μ)
100%	0.1 M	0.20 X 10^{-3}	0.189352 X 10^{-3}	2.07352
	0.075 M	0.15 X 10^{-3}	0.141772 X 10^{-3}	2.13696
	0.050 M	0.1 X 10^{-3}	0.094192 X 10^{-3}	2.26384
	0.025 M	0.06 X 10^{-3}	0.056128 X 10^{-3}	3.02512
80%	0.1 M	0.14 X 10^{-3}	0.132256 X 10^{-3}	1.50256
	0.075 M	0.13 X 10^{-3}	0.12274 X 10^{-3}	1.8832
	0.050 M	0.1 X 10^{-3}	0.09419 X 10^{-3}	2.26384
	0.025 M	0.06 X 10^{-3}	0.056128 X 10^{-3}	3.02512
70%	0.1 M	0.13 X 10^{-3}	0.1227 X 10^{-3}	1.4074
	0.075 M	0.11 X 10^{-3}	0.103708 X 10^{-3}	1.62944
	0.050 M	0.09 X 10^{-3}	0.084676 X 10^{-3}	2.07352
	0.025 M	0.05 X 10^{-3}	0.046612 X 10^{-3}	2.64448

From **Table-1 to Table-2**, it was observed that the observed conductance (G) and specific conductance (k) were decreases from [MDA] to [EDA] continuously while molar conductance (μ) increases. In [MDA] observed conductance continuously decreases from 0.1M concentration to 0.025M concentration continuously. Same pattern was observed in percentage compositions of the mixture. Specific conductance of [MDA] decreases when the molar concentration and percentage composition of water decreases but the specific conductance increases at the same temperature. In [EDA] it was also observed that molar conductance increases from 0.1M concentration to 0.025M concentration as well as it increases in all percentage compositions. In 100% water molar conductance is highest while it will decreases from 100% to 70% water-ethanol percentage compositions. Molar conductance in 100% water is highest in all molar concentrations. Above results showed that [MDA] and [EDA] can give good medicinal activities. Same patterns of observed conductance, molar conductance and specific conductance were observed for [EDA]. These results throw light on pharmacokinetics of [MDA] and [EDA]. During this investigation it was observed that the molar conductance of [MDA] is more than [EDA] which clearly indicates the pharmacokinetic effect of [MDA] is comparatively good than [EDA]. It means that the absorption, transformation and metabolism of [MDA] is better than [EDA], so [MDA] possesses best metabolic activity than [EDA].

The specific constant (Ksp), log (Ksp) and thermodynamics parameter viz. change in free energy (ΔG), change in entropy (ΔS) and change in enthalpy (ΔH) of [MDA] and [EDA] were determined by known literature method at various molar concentration, percentage compositions and temperatures and result are cited in **Table 1** to **Table 8**.

Table 3 : Conductometric Measurements of [MDA] at different concentration					
Determination of Ksp, log Ksp, ΔG,ΔH and ΔS at different Concentrations at 303.15 K					
SYSTEM: [MDH]			**MEDIUM - 100% WATER**		
Conc. (M)	**Ksp**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
0.100	0.07979	-1.02091	5749.358	-580158	-1953.05
0.075	0.054843	-1.14585	6467.024	-580158	-1955.44
0.050	0.029895	-1.32194	7478.517	-580158	-1958.81
0.025	0.004948	-1.62297	9207.676	-580158	-1964.57

Table 4 : Conductometric Measurements of [MDA] at different concentration					
Determination of Ksp, log Ksp, ΔG,ΔH and ΔS at different Concentrations at 303.15 K					
SYSTEM: [MDA]			**MEDIUM - 80% WATER**		
Conc. (M)	**Ksp**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
0.100	0.059832	-1.11782	6306.023	-580158	-1954.9
0.075	0.039874	-1.24276	7023.689	-580158	-1957.25
0.050	0.019916	-1.41885	8035.182	-580158	-1960.67
0.025	-4.2E-05	-1.71988	9764.341	-580158	-1966.43

Table 5 : Conductometric Measurements of [MDA] at different concentration					
Determination of Ksp, log Ksp, ΔG,ΔH and ΔS at different Concentrations at 303.15 K					
SYSTEM:MOLECULE [MDA]			**MEDIUM - 70% WATER**		
Conc. (M)	**Ksp**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
0.100	0.049853	-1.17581	6639.137	-580158	-1956.01
0.075	0.03239	-1.30075	7356.803	-580158	-1958.4
0.050	0.014927	-1.47684	8368.296	-580158	-1961.78
0.025	-0.00254	-1.77787	10097.46	-580158	-1967.54

Table 6: Conductometric Measurements of [EDA] at different concentration					
Determination of Ksp, log Ksp, ΔG,ΔH and ΔS at different Concentrations at 303.15 K					
SYSTEM:MOLECULE [EDA]			**MEDIUM - 100% WATER**		
Conc. (M)	**Ksp**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
0.100	3.905965	0.573946	-3411.73	-580158	-1922.51
0.075	2.924472	0.449008	-2694.07	-580158	-1924.9
0.050	1.942983	0.272916	-1682.57	-580158	-1928.27
0.025	0.961491	-0.02811	46.58543	-580158	-1934.04

Table 7: Conductometric Measurements of [EDA] at different concentration					
Determination of Ksp, log Ksp, ΔG,ΔH and ΔS at different Concentrations at 303.15 K					
SYSTEM:LIGAND [EDA]			**MEDIUM - 80% WATER**		
Conc. (M)	**Ksp**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
0.100	3.120772	0.477036	-2855.07	-580158	-1924.36
0.075	2.335579	0.352098	-2137.4	-580158	-1926.76
0.050	1.550386	0.176006	-1125.91	-580158	-1930.13
0.025	0.765193	-0.12502	603.2504	-580158	-1935.89

Table 8 : Conductometric Measurements of [EDA] at different concentration					
Determination of Ksp, log Ksp, ΔG,ΔH and ΔS at different Concentrations at 303.15 K					
SYSTEM:MOLECULE [EDA]			**MEDIUM - 70% WATER**		
Conc. (M)	**Ksp**	**Log Ksp**	**ΔG**	**ΔH**	**ΔS**
0.100	2.728176	0.419044	-2521.95	-580158	-1925.47
0.075	2.041132	0.294106	-1804.29	-580158	-1927.87
0.050	1.354088	0.118014	-792.795	-580158	-1931.24
0.025	0.667044	-0.70704	936.3644	-580158	-1937

From **Table-3** to **Table-8** it was observed for these molecules Ksp, log Ksp, ΔH and ΔS decreases continuously while ΔG increases when we go from 0.1M concentration solution to 0.025M concentration. Same pattern was observed in percentage composition of the mixture i.e. these thermodynamic parameters are highest in 100% water while least in 70% water-ethanol solvent. In [EDA] the values of all thermodynamic parameter as well as Ksp and log Ksp are the greatest than [MDA].

IV. CONCLUSION:

From this investigation it is clear that various functional groups such as electron donating, electron withdrawing, acidic, basic and various functional groups present in the molecule directly affect conductance, specific conductance, molar conductance, Ksp, ΔH, ΔS and ΔG values of that molecule. The structure of the molecule as well as nature of that molecule directly affects these parameters. The temperature molar concentrations and percentage compositions are also responsible for changing the values of these parameters. The solute (molecule)-solvent interactions, solvent-solvent interactions, solvent-solvent-solute interactions and solute-solute-solvent interactions are another factor which directly hamper these parameters. The internal geometry as well as internal and intra hydrogen bonding affect these parameters.

During this investigation it was also observed that the molar conductance of [MDA] is highest than [EDA] which clearly indicates the molecule effect of [MDA] is comparatively more than [EDA].

V. DISCLOSURE OF CONFLICT OF INTEREST:

Authors wish to state that there is no conflict of interest on this work.

VI. REFERENCES

[1]. Tayade D.T., Waghmare S.A., Am. J. Pharm, Res., 6(3), 2016, 605-612.
[2]. Tayade D.T., BhagwatkarA.K., D.M. Nagrik, J. App. Chem., 2(4), 2013, 993-997.
[3]. Tayade D.T., Mohammad F.Z., Ind. J. Pharma. Sci. Res., 4(4), 2014, 1-3.
[4]. Tayade D.T., Thombare R.D., Eur. J. Pharm. Med. Res., 3(3), 2016, 443-446.
[5]. Lunge M.S., Shaikh R.S., Tayade D.T., Int. J. Adv. Res., 4(1), 2016, 908-912.
[6]. Tayade D.T., Padhen S.S., Eur. J. Pharm. Med. Res. 3(8), 2016, 538-540.
[7]. Tayade D.T., Kale P.R., Int. J. App. Res., 3(3), 2016, 370-374.
[8]. Tayade D.T., Ingole S.P., Eur. J. Pharm. Med. Res., 3(7), 2016. 214-219.
[9]. Tayade D.T., Raghuwanshi M.R., Bhagwatkar A.K., Aswale S.R., Canadian Int. J. Chem., 3(2), 2011, 74-78.
[10]. Murhekar M. M., Padghan P.D., Mhaske S.S., Khadsan R.E., Der pharma Chemica, 2011, 396-399.
[11]. Paranjpe M.G., J. Ind. Chem. Soc., 4(10), 1996, 42-45.
[12]. Chigwada T. R., Chikwana E., Ruwana T., Olagunju O., J. of Phys. Chem. 4,111(45), 2007, 11552-11561.
[13]. Isankar R. D., Tayade D. T., Journal of medicinal chemistry and molecule discovery, 2017, 02, 541-545.
[14]. Bodkhe P. S., WadekarA.B. IsankarR.D. and TayadeD.T., Journal of chemistry and chemical sciences,2019, 9(2), 45-48.
[15]. Tayade K. D., Pund D. A., Isankar R. D., Patil S. U., Journal of Medicinal chemistry and Molecule discovery, 2016, 1, 15-19.
[16]. Tayade D.T., Bhagwatkar A.K., Int. J. of Pharm Pharmaceutical Sci Res, 3(3), 2013, 91-93.
[17]. Sing A.K., Mislıra G., Joyti K., J. App. Pharm. Sci., 01(5), 2011, 44-49.
[18]. Ekhallas N., J Am. Sci., 6(8), 2010, 54-57.
[19]. Sharma P.C., Kharb R., Yar M.S., Kaur P., Int. J. Pharm Sci. Res. 2(4), 2011. 758-771.
[20]. Padghan P. D., Baldaniya B. B., Khadson R. E., Mhaske S. S.Der Pharma Chemica, 3(6), 2011, 243-246.
[21]. S.Chakraborty, D.Shukla, A.Jain,B.Mishra and S.Singh, J.Coll.Int.Sci.,355,242-249,(2009).
[22]. E. A. Gomaa, B. M. Al-Jahdalli, Conductometric Studies of Ionic Association of Divalent Asymmetric Electrolyte Cu(NO3)2 with Kryptofix -22 in Mixed (MeOH-DMF) Solvents at Different Temperatures, American Journal of Condensed Matter Physics, Vol. 2 No. 1, 2012, pp. 16-21. doi: 10.5923/j.ajcmp.20120201.03.
[23]. W.A.L.Izonfuo, C.C.Obunwa, Ind.J.Chem.,38A,939,(1999).
[24]. G.C.Bag, N.M.Singh, N.R.Singh, J.Ind.Chem.Soc.,77,146,(2000).
[25]. N.Dubey, J. Surface Sci. Technol., 24, 139-148, (2008).
[26]. A.B. Wadekar , D. T. Tayade, [2016], Conductometric Study of Substitutedthiocarbamidonaphthols in 70% Ethanol– Water Mixture at Different Molar Concentrations at Constant Temperature, International Journal of Science and Research 5(1),678-680
[27]. Agnieszka Boruń, Conductance and ionic association of selected imidazolium ionic liquids in various solvents: A review, Journal of Molecular Liquids, 276,2019,214-224, https://doi.org/10.1016/j.molliq.2018.11.140.