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## Conductometric studies of 1, 3, 5 –triazinothiocarbamide at different concentration and temperature

DD Sonone, ME Shelke\*, DT Tayade

*Department of Chemistry, Government Vidarbha Institute of Science and Humanities, Amravati, Maharashtra, India.*

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### Abstract

Conductivity plays vital role in drug diffusion. Thermodynamic parameters affected by substituents of drug. Thermodynamic parameters of 1, 3, 5 –triazinothiocarbamide (1a) have been investigated by using conductometrically carried out at different molar concentrations. This work highlights investigation of  $G$ ,  $K$  and  $\mu$  values. The thermodynamic parameters viz.  $\Delta H$ ,  $\Delta S$  and  $\Delta G$  for ion pair formation determine from the value of ion association constant. This technique is suitable and accurate to study of pharmacokinetics and pharmacodynamics parameters.

**Keywords:** Conductometric measurements; Thermodynamic parameters; Pharmacokinetics; Pharmacodynamics; S-triazines

### 1. Introduction

The conductometric measurement is a key of biopharmaceutical parameter responsible for the effective bioavailability and good in vitro and in vivo correlation which gives useful information regarding the permeability of drug. Improvement of solubility and dissolution rate and oral bioavailability of poorly water-soluble drugs are still the challenging aspects for the pharmaceutical technologists [1]. One of the safest methods of solubilisation is hydrotropic solubilization and by the addition of hydrotropic agents the aqueous solubilisation of insoluble drugs can be achieved. Many researchers highlighted the effect of the solubility enhancers (hydrotropic agents) [2] and hence improved stability of the drug but no detailed explanation is available relating to the improvement phenomena.

Conductometric measurements like other transport properties of electrolyte provide useful information about solute-solute and solute-solvent interactions. These interactions have been studied in aqueous and non-aqueous solutions by many workers [3]. The correlation between drugs activities and conductivity proved helpful in studying drug-receptor interactions. Thus, the measurement of conductance of an electrolyte in a solution provides an excellent method of obtaining data on solute-solute and solute-solvent interactions. Conductance measurements can provide the information regarding the transport property of the drugs and ion-solvent interactions. These interactions of electrolyte in binary mixtures of two liquids have been studied in terms of  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  of conductometry [4-5]. The conductometric studies of CPHDD and CTMBCD in ethanol-water mixture at different concentrations and at constant temperature done by Jumde and et.al [6]. Tripathy have reported volumetric and viscometric studies on nimesulide in aqueous solutions of four different hydrotropic agents (sodium benzoate, sodium salicylate, sodium bromide and nicotinamide) at different temperatures, so as to highlight the solute-solvent interactions correlating the solubility findings [7]. Conductometric studies of solutes at definite and infinite dilution in a solvent system provide valuable information regarding the ion-ion and ion-solvent interactions. By investigative the molar conductivity, association constants, Walden products of ionic solutions as a function of size, nature, temperature and composition of the solvent,

\* Corresponding author: ME Shelke

Department of Chemistry, Government Vidarbha Institute of Science and Humanities, Amravati, Maharashtra, India.

it is possible to examine the parameters on solute-solvent interactions with the hope of obtaining a better understanding of interactions in solutions [8].

## 2. Experimental

All the chemicals and solvents used for the synthesis were of A.R. grade. The 1, 3, 5 –triazinethiocarbamide was synthesized as described method [9-11]. The justification of the compound was done on the basis of Melting point, alkaline plumbite test, elemental and spectral analysis. The conductometric measurements of 1, 3, 5-Triazinethiocarbamide have been carried out at 0.1M, 0.050M and 0.025M concentrations in water system at variable temperature. The  $G$ ,  $K$ ,  $\mu$  values and the thermodynamic parameters viz.  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  were also determined in 100% water for one drug by changing the concentration of drugs by serial dilution method and keeping the temperature constant. All the solutions of drug were always used a fresh in the present investigation. In 50 ml glass beaker drug solution was taken and it was kept inside the thermostat for 15-20 minutes to attain the thermal equilibrium (27°C). After achieving the thermal equilibrium, the conductivity of that electrolyte was measured.

From the resulted data, observed conductance ( $G$ ), specific conductance ( $k$ ) and molar conductance ( $\mu$ ) and the thermodynamic parameters  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  were calculated and enlisted in Table 1 and 2 which decides the nature and type of the chemical reaction.

## 3. Results and discussion

During these investigation for conductometric measurements of 100%, distilled water was used. In first set 0.1M solution of (1a) was prepared in conductivity water and by serial dilution method 0.050M and 0.025M solutions were prepared. At 30°C, 40°C, 50°C and 60°C the conductance of each solution was measured by Conductivity Bridge. From the data observed conductance ( $G$ ), specific conductance ( $k$ ) and molar conductance ( $\mu$ ) were determined by known literature method and result are cited in table 1 as a conductometric Measurements of 1, 3, 5 – triazinethiocarbamide (1a) at different concentration.

**Table 1** Determination OF  $G$ ,  $k$  and  $\mu$  at different concentrations and 100 % of solution (Water)

Temp. °C	Concentration C (M)	Observed conductance (G)	Specific conductance (k)	Molar conductance ( $\mu$ )
30	0.1 M	$7.84 \times 10^{-3}$	$7.49296 \times 10^{-3}$	74.92964
	0.050 M	$6.39 \times 10^{-3}$	$6.12411 \times 10^{-3}$	79.16813
	0.025 M	$4.69 \times 10^{-3}$	$4.47688 \times 10^{-3}$	86.6376
40	0.1 M	$7.89 \times 10^{-3}$	$7.52294 \times 10^{-3}$	75.2294
	0.050 M	$6.47 \times 10^{-3}$	$6.17312 \times 10^{-3}$	79.94712
	0.025 M	$4.73 \times 10^{-3}$	$4.49562 \times 10^{-3}$	87.5342
50	0.1 M	$7.92 \times 10^{-3}$	$7.53568 \times 10^{-3}$	75.2568
	0.050 M	$6.51 \times 10^{-3}$	$6.19201 \times 10^{-3}$	80.4521
	0.025 M	$4.77 \times 10^{-3}$	$4.52688 \times 10^{-3}$	87.6241
60	0.1 M	$7.97 \times 10^{-3}$	$7.63421 \times 10^{-3}$	76.3421
	0.050 M	$6.57 \times 10^{-3}$	$6.79302 \times 10^{-3}$	80.0137
	0.025 M	$4.83 \times 10^{-3}$	$4.78469 \times 10^{-3}$	86.9968

From **Table-1**, it was observed that the observed conductance ( $G$ ) and specific conductance ( $k$ ) were increases continuously while molar conductance ( $\mu$ ) increases in a random way. S-Triazines observed conductance continuously increases from 0.1M concentration to 0.025M concentration. This is due to the numbers of S- triazines nucleus present in these solutions in 100% water. As molar conductance in 100% water is highest in all molar concentrations hence, this drug conforms pharmacokinetics and pharmacodynamics of the standard drug. These results throw lights on

pharmokinetics of this drug. During this investigation it was observed that the molar conductance is highest which clearly indicates the drug effect of S- triazines. It means that the absorption, transformation and metabolism of S- triazines are better and possesses best drug activity and drug effect.

The specific constant (Ksp), log (Ksp) and thermodynamics parameter viz. change in free energy ( $\Delta G$ ), change in entropy ( $\Delta S$ ) and change in enthalpy ( $\Delta H$ ) were determined by known literature methods at various molar concentration and temperatures and result are cited in table no. 2

**TABLE 2** Determination of Ksp, log Ksp,  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  at different Concentrations and temperature

Temp.	Conc.	Ksp	Log ksp	$\Delta G$	$\Delta H$	$\Delta S$
30°C	0.1	0.36367	-0.21240	-1765.74	382.67166	0.52573
	0.050	0.17622	-0.61928	-3110.01	1236.0654	4.12341
	0.025	0.24600	-0.58004	-2312.12	1072.7634	2.4775
40°C	0.1	0.19634	-0.67132	-3984.08	3243.0553	10.5839
	0.050	0.12892	-0.85654	-4041.20	1042.3245	2.33865
	0.025	0.16521	-0.74231	-4417.43	231.79152	0.79432
50°C	0.1	0.225112	-0.60564	-3754.54	1024.1307	10.2352
	0.050	0.18345	-0.66765	-4082.21	2743.5346	7.43566
	0.025	0.19885	-0.66651	-4087.16	28137.643	90.1883
60°C	0.1	0.23515	-0.59771	-3715.67	--	--
	0.050	0.23484	-0.60104	-3773.93	--	--
	0.025	0.23515	-0.59771	-3715.67	--	--

From **Table 2** it was observed for these drugs, the Ksp, and log Ksp decreases continuously, while  $\Delta H$ ,  $\Delta S$  and  $\Delta G$  increases randomly when we go from 0.1M concentration solution to 0.025M concentration.

#### 4. 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,  $\Delta H$ ,  $\Delta S$  and  $\Delta G$  values of that drug. The structure of the drug as well as nature of that drug directly affects these parameters. The temperature, molar concentrations and percentage compositions are also responsible for changing the values of these parameters. The solute (drug)-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.

#### Compliance with ethical standards

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##### Disclosure of conflict of interest

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

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