Research Paper Chemistry

The thermodynamic studies of substituted heterocyclic compound in ethanol system in the temperature range 303 to 318K.

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ABSTRACT

Densities, viscosities of some substituted heterocyclic drug (Ebastine) in ethanol were measured in the temperature range 303K to 318K. The viscosity was determined by John–Dole equation. The data has been used to calculate Gibb's free energy change (ΔG), entropy change (ΔS), and enthalpy change (ΔH).ΔG and ΔH are negative and ΔS is positive which is indicate the spontaneity of reaction according to thermodynamics.

KEYWORDS : Thermodynamic parameters, Viscosity, density.

Introduction

The substituted heterocyclic drug 4-(4-benzhydryloxy-1-piperidyl)-1-(4-tert-butylphenyl) butan-1-one (Ebastine). Ebastine is beneficial for anti allergic. Ebastine is a second-generation H1 receptor antagonist that is indicated mainly for allergic rhinitis and chronic idiopathic urticaria[1]. Ebastine is a second-generation antihistamine which has been shown to be an effective treatment for both seasonal and perennial allergic rhinitis.[2]

The thermodynamic properties of solution are important in chemistry and biology. Studies of the viscosities of such solutions were among the earliest in the field of solution chemistry. Sondawale have also studied the viscosity at different temperature using 20% dioxane-water and methanol-water mixture[3]. Agrawal et.al. have been studied the thermodynamic parameters from viscosity measurements of ligand in 70% dioxane–water mixture at different temperature[4]. Brent Hawrylak[5] et. al. have studied the enthalpy of activation , Gibb's free energy of activation and entropy of activation of mixture of isomeric butandiols with water in the temperature range 25°C to 45°C. Kapadi[6] et.al. have studied the thermodynamic interaction of 2,3 butanediol in water in the temperature range 303.15 t 318.15 K. Man chai Change[7] has studied the viscosity and thermodynamic parameters of liquid sulfur in temperature range 430K to 650 K. He also studied the equilibrium between sulfur-halogen systems by equilibrium equation. Irina[8] et al studied the Viscosity, density and refractive index of biodiesel and diesel in benzene at different temperature. Sonar[9] et al studied the thermodynamic parameters of derivative of thiabendazole in 1, 4 Dioxane System in the Temperature Range 303 to 323 K.

Therefore the present work is undertaken to make the systematic study of above substituted heterocyclic drug viscometrically at temperature range 303 K. to 318 K. From viscosity and density measurements we planned to study thermodynamic parameters.

Experimental

The present work is a continuation of our systematic experimental studies on the thermodynamic properties of the substituted heterocyclic drug ebastine. The market drug used for this work. The solvent ethanol was used for preparation of drug solution. The density measurements of the pure solvent and the solutions were performed by using specific gravity bottle between 303.00K and 318.00K. The viscometer put in double wall glass cell. For viscosity measurement Ostwald viscometer (10 ml) was used. The constant temperature was maintained by circulating water through the double wall measuring cell, made up of glass. The flow time was also measured by using digital clock (0.01 Sec).

Theory

The relationship between coefficient of viscosity of liquid and temper-

$$\eta_r = A \cdot e^{-\Delta G / RT} \quad \text{---------- (1)}$$

The thermodynamic parameters were calculated by using following equations

$$\Delta G = -2.303\ R \times \text{Slope} \quad \text{---------- (2)}$$

$$\log \eta_{r2} / \eta_{r1} = [\Delta H / 2.303R]\ [T_2 - T_1 / T_1 T_2] \quad \text{----------(3)}$$

$$\Delta S = (\Delta H - \Delta G) / T \quad \text{----------(4)}$$

Result and discussion

The rise of the temperature is accompanied by a decrease of the viscosity of the solution. The rise of the temperature is accompanied by a decrease of the density of the solution. The table-1 shows values of viscosity and density at different temperature. The thermodynamic functions of viscous flow were estimated from the dynamic Viscosity values. Flow process is governed by the ability of molecule to move into the prepared hole and the readiness with which the holes are prepared in the liquid.

The values of Gibb's free energy were calculated from the slope of graph by plotting logh Vs 1/T (Fig.1). The values of Gibb's free energy were determine by using equation (2) are given in table -2. The value of Gibb's free energy is negative for system. The values of enthalpy change in reaction were determined by using equation (3).The values of enthalpy is also negative in for given systems. From the values of DG and DH, the reaction is spontaneous and exothermic in nature. The values of entropy change were determined from equation (4). The positive value of entropy change indicates the reaction must be spontaneous process of flipping of molecule over each other. DS were positive due the destruction of hydrogen bond in compounds.

Table-1 Viscosity measurements at various temperatures

Temp.	1/T	Density (Kg/m^3)	Time (Sec.)	η_r	logη_r
Ebastine + Ethanol					
303	3.3003x10^{-3}	8268.1	493	1.3309	0.1242
308	3.2468x10^{-3}	8239.9	468	1.2591	0.1001
313	3.1949x10^{-3}	8221.4	442	1.1866	0.07429
318	3.1447x10^{-3}	8219.3	427	0.3408	-0.4675

Table-2 Values of thermodynamic parameters

Systems	ΔG (J mole^{-1} K^{-1})	ΔH (J mole^{-1} K^{-1})	ΔS (J K^{-1})
Ebastine + Ethanol	-9061.002	-3974.61	16.2505

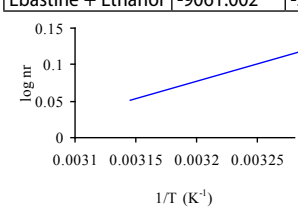

Fig. 1- Plots of log nr Vs 1/T for substituted heterocyclic drug (Ebastine) in ethanol

Conclusion

The viscous flow of the substituted heterocyclic drug in ethanol is thermodynamically spontaneous and exothermic process. Because ΔG and ΔH are negative and ΔS is positive which is indicate the spontaneity of reaction according to thermodynamics.

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