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Viscosity and Density Studies of Drugs in Aqueous Solution and in Aqueous Threonine Solution at 298.15 K

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ABSTRACT

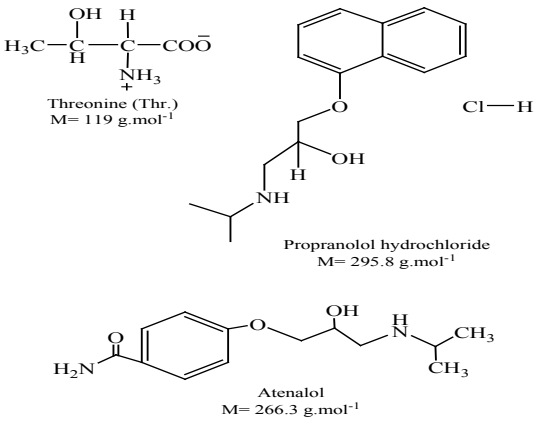
Viscosities (η) and densities (ρ) of atenolol and propranolol hydrochloride in water and in concentrations (0.05 M) and (0.1 M) aqueous solution of threonine have been used to reform different important thermodynamic parameters like apparent molal volumes ϕv partial molal volumes at infinite dilution ϕv^o, transfer volume $\phi v^o(tr)$, the slop S_v, Gibbs free energy of activation for viscous flow of solution $\Delta G^*_{1,2}$ and the B-coefficient have been calculated using Jones-Dole equation. These thermodynamic parameters have been predicted in terms of solute-solute and solute-solvent interaction.

Keywords: L-Threonine, Atenolol, Propranolol hydrochloride, Viscosity, Density.

INTRODUCTION

Drug work in human body is known as pharmacodynamics. The efficiency of a drug depends on its bioavailability[1]. The general reason of low oral bioavailability is due to low solubility of drug molecules. Sometimes, low aqueous soluble drugs require high dosages for the coveted action. Low water solubility of drugs is a serious problem for generic developments. Solubility of most drugs is having poor aqueous. Therefore, the raise of drug solubility and its oral bioavailability is a difficult function for drug evaluation process. Sometimes, some carrier molecules are added to the drugs to increase the solubility[2]. Numerous of works related to volumetric and viscometric properties of drugs have been completed by many researchers[3-5]. Molecular interaction (solute-solute and solute-solvent) have great importance in physical chemistry and geochemistry. Viscosity beta-coefficient, partial molar volumes and apparent molar volumes are advantageous in understanding solute-solvent interactions[6,7]. L-Threonine (abbreviated as Thr.) distributing polar amino acid, is an essential α-amino acids. It was discovered at last of 20 common proteinogenic amino acids with two chiral centers. 4-(2-hydroxy-3-[(1-methylethyl)amino] propoxy)benzeneacetamide is known chemically as atenolol (ATN)[8], is a β1-selective (cavdio selective) adrenorecepter discount drug used for antiangina

therapy to relive symptoms, get better indulgence, and an antiarrhythmic to useful check heartbeat and infections. Atenolol is also used in management of alcohol with drawl, in worry states, headache prophylaxis, increased of metabolism, and tremble[9]. The drug is formal in Indian pharmacopoeia[10]. Isopropyl amino-3-(1-naphthyloxy) propan-2-ol hydrochloride, is known chemically propranolol hydrochloride, is a widely used non-cardio selective beta-adrenergic antagonist and been used for myocardial infarction, arrhythmia, angina pectoris, hypertension, migraine and anxiety[11]. Threonine a polar side chains and exhibits good solubility in water, the nature of solute-solute and solute-solvent interactions have been discussed in terms of the values of $\phi_{v,}$ ϕv^o, S_v and beta-coefficient. Thermodynamic parameters play an important role in detecting the various types of interactions occurring in solution. These are useful in illustrating the nature and effect of solute in solvent, intermolecular interactions and permeation of drug across biological membranes.



EXPERIMENTAL

Amino acid L-threonine obtained from Fluka company is stock solution and used without any further treatment. Atenolol and propranolol hydrochloride were supplied by the state company for drugs industry were medical appliances Samarra Iraq. The viscosity (η) was determined using assuspended-level ubbelohode viscometer described by findly, in a bath controlled to ± 0.01 K for all measurements. Vibrating tube with digital anton parr densimeter (DMA 60/602) according to Shukla *et al.,* in a thermostated bath controlled to ± 0.01 K used to measure densities for all solution.

RESULT AND DISCUSSION

The apparent molal volume (ϕv) is calculated using the following equation[12,13,14].

$$\phi v = \frac{1}{m}\left[\frac{10^3+mM}{\rho} - \frac{10^3}{\rho_o}\right] \quad (1)$$

Where ρ and ρ_o are the densities of solution and solvent respectively, M is molecular weight of solute and (m) is the molality of solution, m is calculated using the following relation:

$$m = 1 / \left(\frac{\rho}{c} - M/10^3\right) \quad (2)$$

Where (C) is the molar concentration. As the plots of ϕv against the molal concentration (m) were linear in the studied concentration range, standard partial molar volume ϕv^o was obtained from the Masson equation[15].

$$\phi v = \phi v^o + S_v m \quad (3)$$

Where ϕv^o is the partial molal volume at infinite dilution which gives information about solute hydrophobicity also a measure of solute-solvent interaction. S_v is slop indicating solute-solute interaction. The Gibbs free energy of activation for viscous flow of solution at a given temperature and composition was measure by basing transition theory is given by equation[16].

$$\Delta G^* = RT\ln\left(\frac{\bar{V}_{1,2}\eta}{hN_A}\right) \quad (4)$$

Where h is planks constant, N_A is Avogadro's number, R is the gas constant and T is the absolute temperature. Volume of mole solution, $\bar{V}_{1,2}$ obtained from the following relation.

$$\bar{V}_{1,2} = (10^3 + mM_2)/\rho\left(\frac{10^3}{M_1} + m\right) \quad (5)$$

Where M_2 and M_1 are the molecular weight for solute and solvent respectively.

The viscosity measurements have been analyzed in terms of Jones-Dole equation[17].

$$\eta_r = \frac{\eta}{\eta_o} = 1 + BC \quad (6)$$

Where η and η_o are the viscosities of solution and solvent respectively and C is the molarity of solution, using Jones-Dole equation, was

calculated viscosity beta-coefficients. The value of B depends upon the nature of solute-solvent interaction which is specific for solute-solvent system and the size of solute. The standard partial molar volume of transfer was obtained from the following relation[18].

$$\phi v^{o}\ (tr) = \phi v^{o}\ (\text{in aqueous threonine}) - \phi v^{o}\ (\text{in water}) \quad (7)$$

The values of $\phi v^{o}(tr)$ and Sv are listed in Table 7 and 8. The values of $\phi v^{o}(tr)$ of drugs in mixed liquids (threonine + water) are higher than those in aqueous solution, $\phi v^{o}(tr)$ are positive for all solutions studied and S_v are positive which indicates ion-ion interaction is greater than post-micellar region. The beta-coefficients measure the shape effects, the size as well as the structural effect induced by solute-solvent interaction. It can be seen from Tables (1-6) that all the viscosity B-coefficients for drugs are positive, this may be understanding in expressing of the solute-solvent interaction.

Table 1: Molarity, molality, density, viscosity, apparent molal volume, Gibbs free energy of activation for viscous flow, relative viscosity and parameters of Jones-Dole coefficients of atenolol in aqueous solution at 298.15 K

C (mol. L^{-1})	M (mol. Kg^{-1})	ρ (gm. cm^{-3})	η(cp)	ϕv(cm^3. mol^{-1})	ΔG^* (J. mol^{-1})	η_r	Jones-Dole beta-coefficient
0.0000	0.0000	0.99705	0.89039	-	-	-	2.7846
0.005	0.0050198	0.99733	0.95941	200.89778	61005	1.07752	
0.006	0.0060244	0.99744	0.962627	201.90081	61014	1.08113	
0.007	0.0070308	0.9975	0.969056	202.61638	61031	1.08835	
0.008	0.0080368	0.99755	0.97455	204.406406	61045	1.09452	
0.009	0.0090435	0.99759	0.97874	206.91372	61057	1.09923	
0.01	0.0100506	0.99763	0.98042	208.919201	61061	1.10111	
0.02	0.020038	0.9981	1.00655	214.15282	61131	1.13046	
0.03	0.03029	0.99843	1.031864	220.9535	61198	1.15889	
0.04	0.040492	0.99857	1.05174	228.97696	61252	1.18121	
0.05	0.050744	0.99865	1.07546	234.99362	61313	1.20785	

Table 2: Molarity, molality, density, viscosity, apparent molal volume, Gibbs free energy of activation for viscous flow, relative viscosity and parameters of Jones-Dole coefficients of propranolol hydrochloride in aqueous solution at 298.15 K

C (mol. L^{-1})	M (mol. Kg^{-1})	ρ (gm. cm^{-3})	η(cp)	ϕv (cm^3. mol^{-1})	ΔG^* (J. mol^{-1})	η_r	Jones-Dole beta-coefficient
0.0000	0.0000	0.99705	0.89039	-	-	-	3.5047
0.005	0.0050204	0.99742	1.03175	224.96221	61186	1.15876	
0.006	0.0060259	0.99748	1.034838	224.8014	61194	1.16223	
0.007	0.007032	0.99755	1.04481	225.04145	61218	1.17343	
0.008	0.0080382	0.99761	1.051738	226.47684	61235	1.18121	
0.009	0.009045	0.99767	1.05554	227.58442	61244	1.18548	
0.01	0.0100527	0.99772	1.058166	229.48006	61251	1.18843	
0.02	0.020155	0.99823	1.089348	237.50229	61329	1.22345	
0.03	0.030042	0.99859	1.1144481	244.73276	61391	1.25164	
0.04	0.040535	0.99864	1.150704	256.80856	61477	1.29236	
0.05	0.05082	0.99872	1.179206	263.17909	61545	1.32437	

Table 3: Molarity, molality, density, viscosity, apparent molal volume, Gibbs free energy of activation for viscous flow, relative viscosity and parameters of Jones-Dole coefficients of atenolol in (0.05 M) aqueous solution of threonine at 298.15 K

C (mol. L^{-1})	M (mol. Kg^{-1})	ρ (gm. cm^{-3})	η(cp)	ϕv (cm^3. mol^{-1})	ΔG^* (J. mol^{-1})	η_r	Jones-Dole beta-coefficient
0.0000	0.0000	1.01235	1.09357	-	-	-	0.1674
0.1	0.10333	1.01348	1.29517	251.8892	66137	1.18435	
0.2	0.20806	1.0145	1.31952	252.4325	66217	1.206623	
0.3	0.32069	1.01537	1.34275	253.1074	66295	1.2278651	
0.4	0.43981	1.01602	1.37257	253.9881	66386	1.25513	
0.5	0.56588	1.01673	1.38865	254.3983	66455	1.26983	
0.6	0.699904	1.01704	1.41917	255.3299	66544	1.29774	
0.7	0.84296	1.01726	1.43745	256.1226	66614	1.31446	
0.8	0.99473	1.01728	1.46028	256.964	66694	1.33533	
0.9	1.15735	1.01731	1.49297	257.6075	66789	1.36523	
1.0	1.33147	1.01735	1.50993	258.1123	66859	1.38073	

Table 4: Molarity, molality, density, viscosity, apparent molal volume, Gibbs free energy of activation for viscous flow, relative viscosity and parameters of Jones-Dole coefficients of atenolol in (0.1 M) aqueous solution of threonine at 298.15 K

C (mol. L^{-1})	M (mol. Kg^{-1})	ρ (gm. cm^{-3})	η(cp)	ϕv (cm^3. mol^{-1})	ΔG* (J. mol^{-1})	η_r	Jones-Dole beta-coefficient
0.0000	0.0000	1.01458	1.10257	-	-	-	0.1759
0.1	0.10115	1.01525	1.31328	255.86944	66167	1.19111	
0.2	0.20777	1.01591	1.33693	256.26352	66246	1.21256	
0.3	0.32034	1.01639	1.35863	256.52647	66322	1.23224	
0.4	0.43941	1.01684	1.38817	256.9044	66412	1.25904	
0.5	0.565572	1.01721	1.40025	257.2887	66435	1.26999	
0.6	0.69971	1.01728	1.42731	258.0379	66557	1.29453	
0.7	0.84246	1.01731	1.45057	258.62898	66637	1.31563	
0.8	0.99468	1.01732	1.47854	259.09737	66724	1.34099	
0.9	1.157303	1.01733	1.52403	259.4657	66840	1.38225	
1.0	1.331434	1.01735	1.55954	259.9546	66939	1.41446	

Table 5: Molarity, molality, density, viscosity, apparent molal volume, Gibbs free energy of activation for viscous flow, relative viscosity and parameters of Jones-Dole coefficients of propranolol hydrochloride in (0.05 M) aqueous solution of threonine at 298 .15 K

C (mol. L^{-1})	M (mol. Kg^{-1})	ρ (gm. cm^{-3})	η(cp) (cm^3. mol^{-1})	ϕv	ΔG* (J. mol^{-1})	η_r	Jones-Dole beta-coefficient
0.0000	0.0000	1.01674	1.11425	-	-	-	0.2137
0.1	0.100985	1.01983	1.33918	260.53875	65943	1.20187	
0.2	0.207551	1.02278	1.36556	261.227123	66078	1.22554	
0.3	0.320202	1.02565	1.40066	261.72403	66128	1.25704	
0.4	0.439614	1.02821	1.41347	262.727004	66184	1.26854	
0.5	0.56655	1.03044	1.45717	263.98106	66305	1.30776	
0.6	0.70165	1.03261	1.4932	264.91539	66407	1.34009	
0.7	0.84589	1.03459	1.50444	265.84971	66468	1.35018	
0.8	0.999713	1.03641	1.56044	266.5829	66598	1.40044	
0.9	1.165999	1.03809	1.58841	267.60016	66691	1.42554	
1.0	1.34447	1.03959	1.64204	268.45699	66819	1.47367	

Table 6: Molarity, molality, density, viscosity, apparent molal volume, Gibbs free energy of activation for viscous flow, relative viscosity and parameters of Jones-Dole coefficients of propranolol hydrochloride in (0.1M) aqueous solution of threonine at 298.15 K

C (mol. L^{-1})	M (mol. kg^{-1})	ρ (gm. cm^{-3})	η(cp)	ϕv (cm^3. mol^{-1})	ΔG* (J. mol^{-1})	η_r	Jones-Dole beta-coefficient
0.0000	0.0000	1.01824	1.13057	-	-	-	0.2321
0.1	0.10089	1.02071	1.39121	266.24253	65999	1.23054	
0.2	0.20749	1.02305	1.40741	266.88177	66066	1.24487	
0.3	0.32037	1.02515	1.43717	267.88028	66157	1.27119	
0.4	0.44019	1.02701	1.46598	268.9692	66247	1.29667	
0.5	0.56767	1.02869	1.49854	269.97606	66343	1.32547	
0.6	0.70371	1.03011	1.52109	271.07243	66424	1.34542	
0.7	0.84935	1.03122	1.60653	272.27648	66646	1.42099	
0.8	0.99446	1.03221	1.6393	273.35163	66697	1.44998	
0.9	1.173617	1.03308	1.67062	274.30782	66794	1.47768	
1.0	1.356134	1.03319	1.69098	275.81896	66903	1.49569	

Table 7: Limiting, partial molal volume, slop and partial molal volume of transfer at infinite dilution of atenolol at 298.15 K

Conc.	ϕv^o	S_v	ϕv^o(tr) (cm^3. mol^{-1})
0%	198.8	732.13	-
0.05 M	251.48	5.2735	52.68
0.1 M	255.49	3.467	56.68

Table 8: Limiting, partial molal volume, slop and partial molal volume of transfer at infinite dilution of propranolol hydrochloride at 298.15 K

Conc.	ϕv^o	S_v	ϕv^o(tr)(cm^3. mol^{-1})
0%	219.32	881.41	-
0.05 M	259.94	6.6078	40.62
0.1 M	265.49	7.7197	46.17

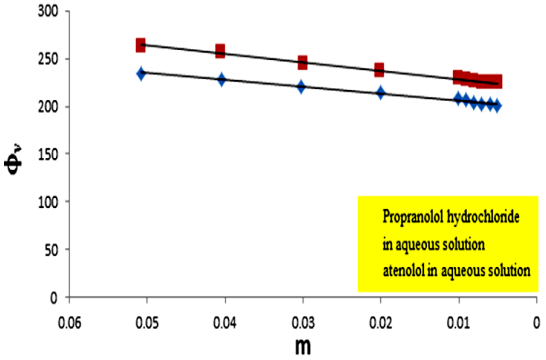


Fig. 1. Plots of ϕv versus (m) for (□) propranolol hydrochloride and (♦) atenolol in aqueous solution at 298.15 K

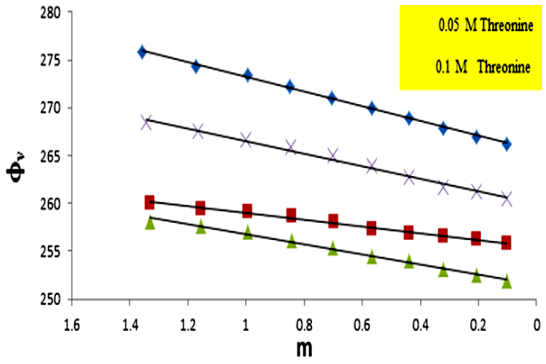


Fig. 2. Plots of ϕv versus (m) for (X) propranolol hydrochloride, (□) atenolol in 0.05 M threonine and (♦) propranolol hydrochloride, (▲) atenolol in 0.1 M threonine

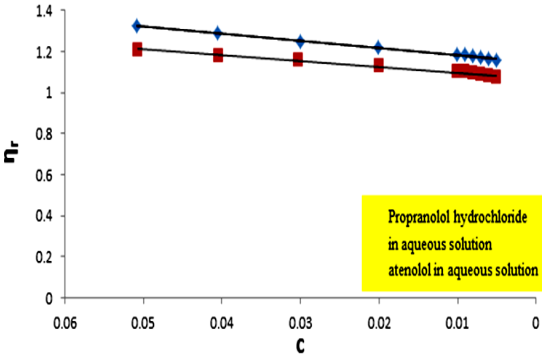


Fig. 3. Plots of η_r versus (c) for (♦) propranolol hydrochloride and (□) atenolol in aqueous solution at 298.15 K

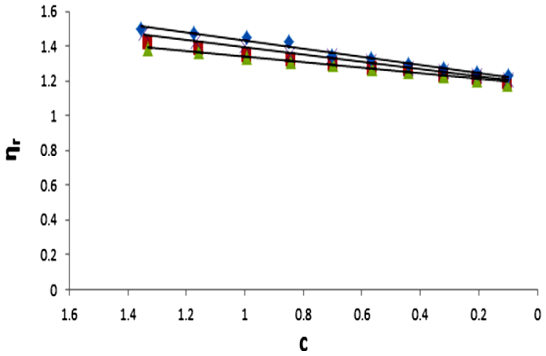


Fig. 4. Plots of η_r versus (c) for (X) propranolol hydrochloride, (▲) atenolol in 0.05 M threonine and (♦) propranolol hydrochloride, (□) atenolol in 0.1 M threonine at 298.15 K

CONCLUSION

The density and viscosity of atenolol and propranolol hydrochloride in water and in concentrations (0.05 M and 0.1 M) aqueous solution of threonine are measured. Different thermodynamics parameters such as ϕv^o, $\phi v^o(tr)$, ΔG^* and viscosity beta-coefficient are calculated, the results show the existence of strong solute-solvent interactions.

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Conflict of interest

On behalf of all coauthors, I certify that all of the materials in this manuscript have no financial interest or non-financial interest with any organization, person, or any entity.

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