



Volumetric and viscometric studies of some drugs in aqueous solutions at different temperatures

Sudhakar S. Dhondge^{a,*}, Sangesh P. Zodape^b, Dilip V. Parwate^c

^a Department of Chemistry, S.K. Porwal College, Kamptee, Nagpur 441 002, India

^b Department of Chemistry, N.Y.S.S. College of Engineering and Research, Nagpur 440 110, India

^c Department of Chemistry, R.T.M. Nagpur University, Nagpur 440 033, India

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ABSTRACT

Density and viscosity measurements are reported for aqueous solutions of the drugs like Metformin hydrochloride (MH), Ranitidine hydrochloride (RH) and Tramadol hydrochloride (TH) at different temperatures $T = (288.15, 298.15, \text{ and } 308.15) \text{ K}$ within the concentration range $(0 \text{ to } 0.15) \text{ mol} \cdot \text{kg}^{-1}$. The density and viscosity data are used to obtain apparent molar volume of solute (ϕ_V) and relative viscosity (η_r) of aqueous solutions at different temperatures. The limiting apparent molar volume of solute (ϕ_V^0), limiting apparent molar expansivity (ϕ_E^0), thermal expansion coefficient (α^*), hydration number (n_h), Jones–Dole equation viscosity *A* and *B* coefficients, experimental slope (S_V) at different temperatures, and temperature coefficient of *B* i.e. (dB/dT) at $T = 298.15 \text{ K}$ were also obtained. The results obtained have been interpreted in terms of solute–solvent and solute–solute interactions and structure making/breaking ability of solute in the aqueous solution.

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1. Introduction

Understanding the action of drugs in aqueous solution has been a subject of research as they exert their activity by interaction with biological membrane. Physicochemical and thermodynamic investigations also attract the inquisitive minds of researchers owing to the important role that drugs play. Physicochemical and thermodynamic investigations play an important role in understanding the nature and the extent of the patterns of molecular aggregation that exist in binary liquid mixtures and their sensitivities to variations in composition and the molecular structure of the pure components [1]. In biophysical chemistry, drug–macromolecular interaction is an important phenomenon involving a complex mechanism [2]. Since most of the biochemical processes occur in aqueous media, the studies on the thermodynamic and transport properties of drugs in the aqueous phase provide useful information in pharmaceutical and medicinal chemistry [3]. The drug–water molecular interaction and their temperature dependence play an important role in the understanding of drug action. Volumetric and viscometric properties provide valuable clues for solute–solvent interactions in the solution phase. Such results can be helpful in predicting the absorption of drugs and transport of drugs across the biological membranes. Therefore, it may be interesting to investigate variation of their properties with temperature for understanding the mechanism of drug action. The detailed literature survey reveals that ther-

modynamic and transport properties of the above mentioned drugs in aqueous medium are scarce. This prompted us to investigate the thermodynamic and transport properties of three pharmacologically significant aqueous solutions of selected drugs, namely, Metformin hydrochloride (MH), Ranitidine hydrochloride (RH), and Tramadol hydrochloride (TH). MH is used for treating type II diabetes in adults and children, RH is commonly used in treatment of peptic ulcer disease (PUD) and gastroesophageal reflux disease and TH is used to treat moderate to moderately severe pain and most types of neuralgia, including trigeminal neuralgia. The present work represents the continuation of a systematic investigation of the volumetric and transport properties of drugs viz., MH, RH, and TH in aqueous solutions at various temperatures $T = (288.15, 298.15, \text{ and } 308.15) \text{ K}$. The derived parameters such as apparent molar volume of solute (ϕ_V), experimental slopes (S_V) of $(\phi_V - A_V(m)^{1/2})-m$ curves (where m is molality of solution), limiting apparent molar volume of solute (ϕ_V^0), limiting apparent molar expansivity (ϕ_E^0), thermal expansion coefficient (α^*), hydration number (n_h), the temperature coefficient of apparent molar thermal expansivity ($\partial^2 \phi_V^0 / \partial T^2$), Jones–Dole equation viscosity *A* and *B*-coefficients and temperature coefficient of *B* i.e. (dB/dT) at $T = 298.15 \text{ K}$ have been obtained. The results of all these are presented and discussed below.

2. Experimental

The compounds Metformin hydrochloride (CAS No. 657-24-9), Ranitidine hydrochloride (CAS No. 71130-06-8), and Tramadol hydrochloride (CAS No. 22204-88-2) used in this study have been

* Corresponding author. Tel.: +91 9822560057.

E-mail address: s_dhondge@hotmail.com (S.S. Dhondge).

procured from Arco Life Science Pharmaceutical. All the compounds were of 0.999 mass fraction purity. The purity was checked by mass spectral analysis (LC–MS). The details are also given in table 1. The above compounds were dried in a vacuum oven and then stored in desiccator under vacuum over fused calcium chloride before use. They were used without any further purification. All the solutions were prepared in freshly prepared doubly distilled water on a molality basis and converted to the molarity scale when required, using density data at different temperatures. A Mettler balance having a precision of 0.1 mg was used for weighing. The temperatures $T = (288.15 \text{ and } 298.15) \text{ K}$ of experimental water bath were maintained constant up to $\pm 0.002 \text{ K}$ by circulating the coolant liquid from the ultra-cryostat type MK-70 (accuracy $\pm 0.02 \text{ K}$) and $T = (308.15 \pm 0.002) \text{ K}$ by circulating the thermostatted liquid from Julabo cryostat which maintains the temperature constant to $\pm 0.01 \text{ K}$ in the cryostat. The densities of the solutions were measured at different temperatures using Lypkin's modified bicapillary Pycnometer (volume $\approx 31 \text{ cm}^3$). The details are given elsewhere [4]. The uncertainty in density measurements was confirmed by measuring the densities of dilute aqueous NaCl solutions at $T = (288.15, 298.15, \text{ and } 308.15) \text{ K}$. The experimental densities agreed well with the literature to $\pm 5 \cdot 10^{-2} \text{ kg} \cdot \text{m}^{-3}$ [5].

Viscosity measurements were made using an Ubbelohde viscometer suspended in the thermostatic bath having approximately 35 dm^3 capacity. The details are given elsewhere [6]. The flow times of water for the Ubbelohde viscometers are 1246.4 s, 979.7 s, and 796.7 s (viscometer-I) and 1313.6 s, 1029.4 s, and 838.6 s (viscometer-II) at $T = (288.15, 298.15, \text{ and } 308.15) \text{ K}$ respectively. The time was monitored using a stopwatch with least count of 0.1 s. All the flow time measurements reported in this work are averaged over three separate measurements of the same solutions. Viscometers were calibrated by measuring viscosity of aqueous NaCl solutions of different concentrations at $T = (288.15, 298.15, \text{ and } 308.15) \text{ K}$. Our values of relative viscosity (η_r) agreed well with literature [7] to $\pm 0.1\%$.

3. Calculations of derived parameters

The apparent molar volume of the solute in aqueous solution (ϕ_V) has been calculated using the relation:

$$\phi_V = \frac{1000(\rho_0 - \rho)}{m\rho\rho_0} + \frac{M_2}{\rho}, \quad (1)$$

where ρ_0 and ρ are the densities of solvent and solution respectively and m , M_2 are the molality of solution and molar mass of the solute respectively. It is assumed that within the concentration range of compounds studied, hydrolysis if any, is negligible. The data of density and ϕ_V for aqueous solutions of solute at different temperatures are listed in tables 2 to 4. The limiting apparent molar volumes of solute (ϕ_V^0) are normally obtained by smooth extrapolation of ϕ_V – m curves to zero concentration, using the relation:

$$\phi_V = \phi_V^0 + S_V m, \quad (2)$$

where S_V is the slope of ϕ_V – m curves. However, in the present study all solutes are electrolytes and so Debye–Hückel limiting law for volumes has been used i.e.

TABLE 2

The density (ρ)^a, apparent molar volume of solute (ϕ_V), and relative viscosity (η_r)^b of aqueous solutions of solutes $T = 288.15 \text{ K}$.

$m/(\text{mol} \cdot \text{kg}^{-1})$	$10^{-3} \cdot \rho/(\text{kg} \cdot \text{m}^{-3})$	$10^6 \cdot \phi_V/(\text{m}^3 \cdot \text{mol}^{-1})$	η_r
<i>MH</i>			
0.0000	0.99910	124.10	1.0000
0.0309	1.00034	125.42	1.0160
0.0416	1.00077	125.35	1.0197
0.0506	1.00117	124.54	1.0226
0.0608	1.00155	125.10	1.0256
0.0712	1.00190	126.03	1.0290
0.0815	1.00231	125.92	1.0318
0.0922	1.00271	126.10	1.0338
0.1028	1.00321	125.22	1.0367
0.1138	1.00339	127.47	1.0399
0.1207	1.00371	126.93	1.0422
0.1527	1.00489	127.06	1.0510
<i>RH</i>			
0.0000	0.99910	261.90	1.0000
0.0202	1.00092	260.45	1.0231
0.0306	1.00178	262.74	1.0337
0.0407	1.00269	261.88	1.0379
0.0488	1.00332	263.44	1.0482
0.0602	1.00433	262.78	1.0538
0.0702	1.00527	261.52	1.0667
0.0813	1.00623	261.46	1.0738
0.0920	1.00713	261.64	1.0817
0.1019	1.00793	262.06	1.0960
0.1149	1.00912	261.20	1.1074
0.1521	1.01215	261.81	1.1390
<i>TH</i>			
0.0000	0.99910	251.30	1.0000
0.0138	0.99975	252.76	1.0162
0.0260	1.00036	251.24	1.0263
0.0298	1.00053	251.68	1.0287
0.0400	1.00104	251.04	1.0422
0.0536	1.00172	250.48	1.0543
0.0604	1.00203	250.78	1.0626
0.0702	1.00251	250.59	1.0701
0.0805	1.00296	251.10	1.0811
0.0903	1.00344	250.87	1.0893
0.0990	1.00381	251.26	1.0969
0.1207	1.00482	251.20	1.1207
0.1511	1.00621	251.18	1.1517

^aStandard uncertainties σ are $\sigma(T) = 0.002 \text{ K}$; $\sigma(m) = 0.0001 \text{ mol} \cdot \text{kg}^{-1}$, and the combined expanded uncertainty $U_{\rho}(\rho) = 0.1 \text{ kg} \cdot \text{m}^{-3}$.

^bStandard uncertainties σ are $\sigma(T) = 0.002 \text{ K}$; $\sigma(m) = 0.0001 \text{ mol} \cdot \text{kg}^{-1}$, and the combined expanded uncertainty $U_{\eta}(\eta) = 0.2\%$.

$$\phi_V = \phi_V^0 + A_V(m)^{1/2} + S_V m, \quad (3)$$

where A_V is the Debye–Hückel limiting slope and it changes with temperature [8]. The limiting values of the apparent molar volume (ϕ_V^0) were obtained by smooth extrapolation of $(\phi_V - A_V(m)^{1/2})$ to zero concentration using the Debye–Hückel limiting law correction at different temperatures. The values of A_V at $T = (288.15, 298.15, \text{ and } 308.15) \text{ K}$ have been taken as 1.697, 1.868, and 2.046 respectively [8]. The values of ϕ_V^0 obtained are listed in table 5.

Limiting apparent molar expansivity (ϕ_E^0) has been computed by using the relation:

$$\phi_E^0 = (\partial\phi_V^0/\partial T). \quad (4)$$

TABLE 1

Specification of chemical samples.

Chemical name	Source	Mass fraction purity	Analysis method
Metformin hydrochloride	Arco Life Science Pharmaceutical, India	>0.999	LC–MS ^a
Ranitidine hydrochloride	Arco Life Science Pharmaceutical, India	>0.999	LC–MS ^a
Tramadol hydrochloride	Arco Life Science Pharmaceutical, India	>0.999	LC–MS ^a

^a Liquid chromatography, mass spectrometry.

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