Research Article

Density and Optical Properties of {Ciprofloxacin Hydrochloride + Aqueous-Ethanol} Mixtures at 30°C

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The paper deals with the calculation of molar refraction (R_M) and polarizability (α) of antibiotic drug ciprofloxacin hydrochloride ($c = 0.001\text{--}0.029\text{ mol}\cdot\text{dm}^{-3}$) solutions in ethanol-water mixtures of different compositions (30, 50, and 70% v/v) from measured density (ρ) and refractive index (n) at 30°C. The effect of drug concentration and composition of ethanol-water mixtures on density and optical properties of drug solutions has been described.

1. Introduction

The knowledge of physiochemical properties of drug solution plays an important role in understanding their physiological actions which is highly dependent upon solution behaviour. Drugs are organic molecules with both hydrophilic and hydrophobic groups due to which they show specific as well as electrostatic interactions. Physiochemical properties like ρ and n of solution are directly related to interactions in solution and are useful for recognition of substance; they confirm purity and concentration of substance. Refractive index along with density is used for investigated intermolecular interactions in solution. Molecular interactions are studied through the measurements of refractive indices of solution [1–3]. n and R_M are useful for getting the valuable information about polarizability of solution [4–8].

Ciprofloxacin is second-generation fluoroquinolone used as an antibiotic that can treat a number of bacterial infections. It is used to treat infections such as infections of bones and joints, endocarditis, gastroenteritis, malignant otitis externa, respiratory tract infections, cellulitis, and urinary tract infections. We have studied the optical properties of aqueous metoprolol succinate and duloxetine solutions [9, 10] and ciprofloxacin + aqueous-glycine solutions [11]. Here we report ρ and n of ciprofloxacin hydrochloride solutions in ethanol-water mixtures of 30, 50, and 70% v/v at 30°C. R_M and α of these solutions are calculated. Various properties

are interpreted in terms of molecular interactions in solution. Present work deals with the molecular interactions and overall structural fitting in the drug in aqueous-ethanol solutions and therefore finds the applications in pharmaceutical and medical sciences. The data of thermodynamic properties is helpful for understanding the drug-water and drug-alcohol interactions.

2. Experimental

The ciprofloxacin hydrochloride monohydrate drug was received as a gift sample from Godavari Drugs Ltd., Nanded (MS), India. Ethanol-water mixtures of 30, 50, and 70% v/v were prepared and drug solutions of different concentrations were prepared in given ethanol-water mixtures. Distilled water was used for preparation of drug solutions. Weighing was done on single pan electronic balance ($\pm 0.001\text{ g}$). ρ were determined using calibrated single capillary pycnometer and n were measured on thermostatically controlled Cyber LAB-Cyber Abbe Refractometer (Amkette Analytics, ± 0.0002 , 1.3000 to 1.7000). Averages of three readings of ρ and n are reported.

3. Results and Discussion

Experimental ρ , n , R_M , and α data of ternary {ciprofloxacin hydrochloride + ethanol-water} systems at 30°C are presented in Table 1.

TABLE 1: ρ , n , R_M , and α of ciprofloxacin hydrochloride in ethanol-water mixtures at 30°C.

c mol·dm ⁻³	ρ g·cm ⁻³	n	R_M cm ³ ·mol ⁻¹	$\alpha \times 10^{-24}$ cm ³
30% v/v				
0.001	0.9644	1.3450	4.632	1.837
0.005	0.9651	1.3455	4.641	1.841
0.009	0.9658	1.3460	4.652	1.845
0.013	0.9671	1.3467	4.661	1.848
0.017	0.9679	1.3474	4.673	1.853
0.021	0.9685	1.3480	4.685	1.858
0.025	0.9692	1.3485	4.695	1.862
0.029	0.9699	1.3490	4.705	1.866
50% v/v				
0.001	0.9363	1.3527	5.527	2.192
0.005	0.9364	1.3530	5.542	2.198
0.009	0.9371	1.3535	5.555	2.203
0.013	0.9377	1.3540	5.569	2.208
0.017	0.938	1.3542	5.580	2.213
0.021	0.9383	1.3547	5.597	2.219
0.025	0.9386	1.3555	5.617	2.228
0.029	0.9389	1.3558	5.630	2.233
70% v/v				
0.001	0.8881	1.3556	6.947	2.755
0.005	0.8888	1.3560	6.963	2.761
0.009	0.8893	1.3570	6.992	2.773
0.013	0.8897	1.3580	7.021	2.784
0.017	0.8906	1.3588	7.042	2.793
0.021	0.8911	1.3596	7.068	2.803
0.025	0.8916	1.3605	7.096	2.814
0.029	0.8919	1.3610	7.119	2.823

ρ and n of solutions increased with drug concentration and ρ decreased and n increased with increase in vol % of ethanol in solution for given drug concentration (Figures 1 and 2). As drug concentration increases, due to the drug-solvent interactions, volume contraction occurs which resulted in increase in density of solution. The ρ and n changes are indicative of intermolecular interaction in solution.

Concentration dependence of n is studied [12] using (1) and respective graphical parameters are reported in Table 2:

$$n = K \times c + n^0, \quad (1)$$

where K is constant which depends on chemical and physical properties of solute (dm³·mol⁻¹), c is molar concentration of drug solution (mol·dm⁻³), and n^0 is refractive index at infinite dilution. Relationship between ρ and n is also studied (Figure 3) and found to be linear ($r^2 > 0.950$).

The parameters R_M and α in Table 1 are determined using the following equations [13–15] and presented in Figures 4 and 5:

$$R_M = \frac{(n_D^2 - 1)}{(n_D^2 + 2)} \times \sum_{i=1}^3 \frac{M_i}{\rho_i}, \quad (2)$$

FIGURE 1: ρ with concentration of drug in ethanol-water at 30°C. FIGURE 2: n with concentration of drug in ethanol-water at 30°C.

where x_i is mole fractions of i th component of mixture and M_i is molecular mass of i -component of mixture and

$$\alpha = \frac{3 R_M}{4 \pi N}, \quad (3)$$

where N is Avogadro's constant (6.023×10^{23} mol⁻¹).

R_M is an electronic polarizability per mole of component which includes contributions from each component. Deviation in R_M is an indication of interactions between components [16]. It is used in QSAR studies for drug design [17]. R_M and α appear as a response to combined effects of intermolecular forces between solute and its surroundings [18]. Use of R_M and α has become increasingly important in the study of drug interaction.

TABLE 2: Graphical parameters from concentration dependence of n .

Binary/ternary system	n^0 at infinite dilution ($c = 0$)	K ($\text{dm}^3 \cdot \text{mol}^{-1}$)	r^2
Drug + 30 vol % E-W	1.3448	0.1479	0.9969
Drug + 50 vol % E-W	1.3525	0.1131	0.9863
Drug + 70 vol % E-W	1.3552	0.2051	0.9940

FIGURE 3: ρ - n relationship for drug in ethanol-water at 30°C. FIGURE 5: α with drug concentration in ethanol-water at 30°C. FIGURE 4: R_M with concentration of drug in ethanol-water at 30°C.

R_M increased slightly with drug concentration and largely with vol % of ethanol in solution which indicates strong drug-solvent interactions [19]. Plots of R_M with concentration of drug for all the systems are found to be linear ($r^2 > 0.995$). R_M is directly proportional to α [20]; hence, α increases and becomes stronger with increase in amount of drug which elucidates structural cause of change in density and existence and modification of molecular interactions. Changes in n_D and R_M indicate tighter packing of drug

molecules and strengthening of drug-solvent interactions at higher concentration. With increase in vol % of ethanol, the packing of drug becomes tighter.

α is related to the intermolecular forces in the system like drug-receptor interactions [16]. It is increased with drug concentration as well as with vol % of ethanol in solution which indicates capability of electronic system of drug molecule to be distorted is increase with drug concentration and vol % of ethanol. Stronger polarizability is introduced to drug solution upon addition of drug in ethanol-water mixtures due to interactions between polar parts of the drug and solvent dipoles. Both R_M and α values of ciprofloxacin in ethanol-water are higher than in aqueous medium [11].

4. Conclusions

The n values of ciprofloxacin in aqueous-ethanol mixtures show linear dependence over drug concentration and density. α increases and becomes stronger with increase in amount of drug due to structural cause of change in density and existence and modification of drug-solvent interactions. Overall results indicated the strengthening of drug-solvent interactions with drug concentration. Capability of electronic system of drug to be distorted is increased with drug concentration and vol % of ethanol.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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References

- [1] R. Belda, J. V. Herraez, and O. Diez, "A study of the refractive index and surface tension synergy of the binary water/ethanol: influence of concentration," *Physics and Chemistry of Liquids*, vol. 43, no. 1, pp. 91–101, 2005.
- [2] I. Banik and M. N. Roy, "Study of solute-solvent interaction of some bio-active solutes prevailing in aqueous ascorbic acid solution," *Journal of Molecular Liquids*, vol. 169, pp. 8–14, 2012.
- [3] J. V. Herraez and R. Belda, "Refractive indices, densities and excess molar volumes of monoalcohols + water," *Journal of Solution Chemistry*, vol. 35, no. 9, pp. 1315–1328, 2006.
- [4] J. G. Baragi, M. I. Aralaguppi, T. M. Aminabhavi, M. Y. Kariduraganavar, and A. S. Kittur, "Density, viscosity, refractive index, and speed of sound for binary mixtures of anisole with 2-chloroethanol, 1,4-dioxane, tetrachloroethylene, tetrachloroethane, DMF, DMSO, and diethyl oxalate at (298.15, 303.15, and 308.15) K," *Journal of Chemical and Engineering Data*, vol. 50, no. 3, pp. 910–916, 2005.
- [5] S. L. Oswal, J. S. Desai, and S. P. Ijardar, "Studies of partial molar volumes of alkylamine in non-electrolyte solvents: I. Alkylamines in hydrocarbons at 303.15 and 313.15 K," *Thermochimica Acta*, vol. 449, no. 1-2, pp. 73–89, 2006.
- [6] D. R. Nagargoje, S. A. Lambe, and M. N. Deshpande, "Viscosity and polarizability measurements of 3-acetyl-6-methyl-(2H)-pyran-2,4-(3H)-dione derivative in different phase systems," *Asian Journal of Chemistry*, vol. 20, no. 7, pp. 5785–5787, 2008.
- [7] K. L. Zhuo, Q. Liu, Y. P. Wang, Q. H. Ren, and J. J. Wang, "Volumetric and viscosity properties of monosaccharides in aqueous amino acid solutions at 298.15 K," *Journal of Chemical and Engineering Data*, vol. 51, no. 3, pp. 919–927, 2006.
- [8] B. Sinha, V. K. Dakua, and M. N. Roy, "Apparent molar volumes and viscosity B-coefficients of some amino acids in aqueous tetramethylammonium iodide solutions at 298.15 K," *Journal of Chemical and Engineering Data*, vol. 52, no. 5, pp. 1768–1772, 2007.
- [9] S. D. Deosarkar and T. M. Kalyankar, "Structural properties of aqueous metoprolol succinate solutions. Density, viscosity, and refractive index at 311 K," *Russian Journal of Physical Chemistry A*, vol. 87, no. 6, pp. 1060–1062, 2013.
- [10] S. D. Deosarkar, S. M. Deoraye, and T. M. Kalyankar, "Temperature and concentration dependences of density and refraction of aqueous duloxetine solutions," *Russian Journal of Physical Chemistry A*, vol. 88, no. 7, pp. 1129–1132, 2014.
- [11] S. D. Deosarkar, M. P. Pawar, P. D. Tawde, and S. M. Deoraye, "Refractive index, molar refraction and polarizability of ciprofloxacin hydrochloride in aqueous-glycine solutions," *International Journal of Chemical Sciences*, vol. 3, no. 2, pp. 830–836, 2015.
- [12] F. Koohyar, A. A. Rostami, M. J. Chaichi, and F. Kiani, "Refractive indices, viscosities, and densities for L-Cysteine hydrochloride monohydrate + D-sorbitol + water, and glycerol + D-sorbitol + water in the temperature range between $T = 303.15$ K and $T = 323.15$ K," *Journal of Solution Chemistry*, vol. 40, no. 7, pp. 1361–1370, 2011.
- [13] A. F. Fucaloro, "Reporting molar refractions," *Journal of Solution Chemistry*, vol. 31, no. 7, pp. 601–605, 2002.
- [14] S. D. Deosarkar, M. L. Narwade, H. G. Jahagirdar, and K. M. Khedkar, "The measurement of molar refraction and polarizability constants of some substituted sulphonic acids at 303 K," *Oriental Journal of Chemistry*, vol. 24, no. 3, pp. 1135–1137, 2008.
- [15] S. S. Yadav, D. Khare, and R. Pande, "Studies on molecular interaction parameters of hydroxamic acids at different temperatures in DMA," *Journal of Molecular Liquids*, vol. 177, pp. 243–251, 2013.
- [16] P. Pacák and Z. Kodejš, "Molar volumes and refractivities of highly concentrated solutions of ammonium and potassium thiocyanates in water and dimethylsulphoxide," *Canadian Journal of Chemistry*, vol. 66, no. 9, pp. 2244–2249, 1988.
- [17] V. Tiwari and R. Pande, "Molecular descriptors of N-arylhydroxamic acids: a tool in drug design," *Chemical Biology and Drug Design*, vol. 68, no. 4, pp. 225–228, 2006.
- [18] M. V. Castillo, M. A. Checa, M. E. Manzur et al., "Experimental study of the dielectric behavior of tinidazole in acetone at 25°C," *Vitae*, vol. 17, no. 3, pp. 299–308, 2010.
- [19] Bhanupriya, R. P. Rajwade, and R. Pande, "Densities, refractive indices and excess properties of N-p-tolylbenzohydroxamic acid in dimethyl sulfoxide at 298.15 to 313.15 K," *Journal of Solution Chemistry*, vol. 38, no. 9, pp. 1173–1181, 2009.
- [20] A. Ali, S. Khan, and S. Hyder, "Volumetric, viscometric, and refractive index behaviour of glycine in aqueous diols at different temperatures," *Journal of the Chinese Chemical Society*, vol. 52, no. 2, pp. 215–222, 2005.