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Solvation behaviour of an antihelmintic drug in aqueous solutions of sodium chloride and glucose at different temperatures

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ABSTRACT

The experimental values of densities (ρ), speeds of sound (u) and relative viscosities (η_r) of piperazine citrate in aqueous solution and in 0.06 mol·kg^{-1} of sodium chloride and D-glucose as a function of concentration have been obtained at T/K = (293.15, 303.15 and 313.15). The thermodynamic parameters such as apparent molar volume (V_ϕ) of solute, isentropic compressibility (κ_s), apparent molar isentropic compressibility (κ_ϕ) of solute, piperazine citrate in water and in aqueous solutions of sodium chloride and D-glucose have been computed using the density and speed of sound data. The limiting apparent molar volume of solute (V_ϕ^0), limiting apparent molar compressibility (κ_ϕ^0) in binary and ternary solution have been obtained using apparent molar volume and apparent molar compressibility data. The limiting apparent molar expansivity (E_ϕ^0) of solute and thermal expansion coefficient (α^*) in both aqueous binary and ternary solutions has been computed. Transfer volumes ($\Delta_{tr}V_\phi^0$) and transfer compressibilities ($\Delta_{tr}\kappa_\phi^0$) of piperazine citrate from water to aqueous solutions of sodium chloride and D-glucose at different temperatures have been obtained. The Jones-Dole viscosity coefficients A, B, D, variation of viscosity B coefficient with temperature i.e. dB/dT, hydration number for aqueous solutions of piperazine citrate and in aqueous solutions of sodium chloride and D-glucose have been determined. The above parameters have been used to throw light on the various interactions occurring between binary and ternary systems.

1. Introduction

Drugs are biologically important macromolecules that have been used since ages for diagnosis, alleviation, treatment, cure or anticipation of diseases in living systems. Nowadays there has been a rampant growth in the development of drug delivery systems for the treatment of diseases. The main concern of these ever changing delivery systems is to increase the efficacy of the drug and to diminish the toxicity of the drug. The action of the drug with the biological membranes is also of prominence. This action of the drug or the affinity of the drug for the membrane can be thought of as a measure of the hydrophobic-hydrophillic interactions in the molecule and can be thought of as an extension to surface activity at the air/solution interface [1]. Water is a universal solvent. It is known of its ubiquity and the striking aspects of it make it a marvellous substance [2]. Also water is the host of many biochemical processes. Thus the study of the thermodynamic parameters of drug in aqueous medium and in the presence of various co-solutes such as carbohydrates, proteins, vitamins, amino acids, nucleosides, nucleotides, and inorganic salts of many ions, enhances the understanding of the molecular interactions of drug molecules [3]. Also the drug water interactions at different temperatures are central to the understanding of drug action in living systems [4]. Physicochemical and thermodynamic investigations are important from the point of view of understanding the nature and the extent of the patterns of the molecular aggregations that exist in binary liquid mixtures and their sensitivities to variations in composition and the molecular structure of the pure components. Piperazine citrate is mainly known for its excellent antihelmintic property. Its mode of action is generally by paralyzing parasites, which allows the host body to easily remove or expel the invading organisms [5]. The neuromuscular effects are thought to be caused by blocking acetylcholine at the myoneural junction.

Electrolytes greatly influence the stability of the biomolecules and are necessary for the balance of the osmotic pressure in the living systems. Sodium chloride is one of the major electrolytes present in the body fluids and affects the metabolic processes. The body fluid contains isotonic solutions of sodium chloride (0.06 mol·kg^{-1}) and so it is worthwhile to examine the action of drug on the body fluid [6]. Apart from the electrolytes, the non-electrolytes also play equally important role in understanding

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the drug action in extra cellular fluids [7]. Polyhydroxy compounds also influence the interactions occurring within the cell and play a major role in stabilizing the native structure of the biomolecules [8]. Thus, the study of the drug interactions with the carbohydrates such as D-glucose is equally important for getting a better view of the pharmacokinetics of the drug with the living system.

A detailed understanding of the solution behaviour of anti-helmintic drug requires information on a variety of thermodynamic parameters. The volumes and compressibilities are two important properties, which can be helpful in the identification of solute-solvent, as well as solute-solute interactions [9]. Studies of the limiting apparent molar volumes of the electrolyte of drug molecules have been useful in understanding their action in vitro. Sufficient studies and investigations with respect to volumes, compressibilities and viscosity have not been executed on the anti-helmintic drug, piperazine citrate. In the present study, we report the densities (ρ), speeds of sound (u) and relative viscosities (η_r) of the aqueous solutions of piperazine citrate and in 0.06 mol·kg^{-1} of sodium chloride and D-glucose as a function of concentration at T/K = (293.15, 303.15 and 313.15) as a function concentration. Using the experimental data, different derived parameters have been computed. The results obtained have been interpreted in terms of solute-solvent and solute-solute interactions.

2. Experimental

2.1. Chemicals

Anhydrous piperazine citrate (CAS No. 144-29-6, mass fraction purity ⩾0.99) was supplied by Arco Life Science Pharmaceutical. The provenances, structures and purity of chemicals have been provided in Table 1. The chemicals were used without further purification. However, they were dried in vacuum oven at T/K = 358.15 for 48 h and then stored in a vacuum desiccator over anhydrous-fused calcium chloride before use. All the solutions were freshly prepared in triple distilled water on a molality basis by using an electronic balance (Shimadzu AUW220D) having precision of ±0.1 mg. For the binary solution of piperazine citrate, water has been used as a solvent and for the ternary solution of piperazine citrate, aqueous solutions of sodium chloride (0.06 mol·kg^{-1}) and D-glucose (0.06 mol·kg^{-1}) have been used as solvents.

2.2. Methods

The density, speed of sound and viscosity measurements of aqueous binary and ternary systems of piperazine citrate at different temperatures T/K = (293.15, 303.15 and 313.15) were performed by means of an automated density and sound velocity meter (Anton Paar DSA 5000M) equipped with rolling-ball viscometer Lovis 2000M/ME. The instrument was calibrated with the certified specific standards namely 'Ultra Pure Water' standards for density, speed of sound and viscosity measurements. An air/water adjustment was performed at temperatures T/K = (288.15–313.15) respectively with ultrapure water sample and with dry air at atmospheric pressure. Before each measurement the instrument was rechecked for its specifications with the help of triple distilled water executing a water check. The results agreed well to the literature values [10].

For the further confirmation of the reliability of the calibration, the instrument was checked by measuring the densities of aqueous sodium chloride solutions at T/K = (288.15, 298.15, 308.15) respectively and an excellent agreement was found with the literature values [11,12]. It was observed that the standard uncertainty in the density is of the order of ±0.05 kg·m^{-3}. For speed of sound measurement, the working frequency of the instrument is 3 MHz and the standard uncertainty was evaluated by using freshly prepared triple distilled water and was compared with the literature values at different temperatures T/K = (288.15–313.15) respectively. Our results agreed well with literature data and the standard uncertainty was found to be equal to 0.5 m·s^{-1}[12]. For the viscosity measurements, the Lovis 2000M/ME instrument was calibrated with the reference liquid (S3, N26, N100 liquid for (1.59, 1.8 and 2.5) mm capillary, respectively) supplied by the Anton Paar Co., Austria and also calibrated by measuring the viscosity of aqueous sodium chloride solution. Experimental results were compared with Stokes and Mills data of (NaCl + Water) at T/K = (288.15–313.15) [13]. The accuracy in the relative viscosity measurements was found to be 1%.

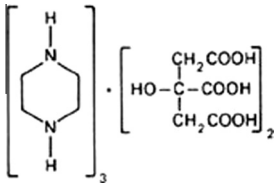
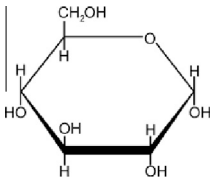
3. Results and discussion

3.1. Volumetric properties

3.1.1. Apparent molar volume

The experimental values of density of aqueous solutions of piperazine citrate and piperazine citrate in 0.06 mol·kg^{-1} aqueous sodium chloride and in 0.06 mol·kg^{-1} aqueous D-glucose solutions at temperatures T/K = (293.15, 303.15 and 313.15) are listed in Table 2. Our values obtained for the density of sodium chloride solution agree well with the values observed by Millero et al. [11] at 298.15 K, Khatun et al. [12] at T/K = (298.15, 303.15, 313.15), Sadeghi et al. [14] at T/K = (293.15, 303.15, 313.15) and those of D-glucose solutions agree well with M. Orian et al. [15],

Table 1
Provenance and mass fraction purity of the chemical samples.

Chemical Name	Provenance	CAS No.	Mass fraction purity[a]	Structure
Piperazine citrate	Arco Lifesciences	144-29-6	⩾0.99	
Sodium chloride	Fischer Scientific	7647-14-5	⩾0.99	Na^+Cl^-
D-Glucose	Fischer Scientific	50-99-7	⩾0.99	

[a] Purity as provided by suppliers.