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Molecular interactions of sodium salicylate in physiological media under the influence of electrolyte/non-electrolyte at different temperatures: Volumetric and acoustic study

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ABSTRACT

Drug interactions in presence of co-solute in aqueous solution have always created an interest in the mind of chemists. The physical properties give an idea of types of interactions taking place in aqueous solution. Volumetric and compressibility are the important physical properties. Keeping this in mind we have measured the densities (ρ) and speeds of sound (u) of sodium salicylate (NaSl) drug (0.01–0.1) mol·kg^{-1} in 0.06 mol·kg^{-1} aqueous sodium chloride solution and 0.06 mol·kg^{-1} myo-inositol as a function of temperature at T = (288.15, 298.15 and 308.15) K and atmospheric pressure. These values have been used to estimate the apparent molar volume of solute (V_ϕ), apparent molar isentropic compressibility (κ_s) of solution and apparent molar isentropic compressibility (κ_ϕ) of solute. The limiting apparent molar expansivity (E^0_ϕ) of solute and coefficient of thermal expansion (α^*) of sodium salicylate in aqueous binary and ternary solutions have also been obtained. Limiting values of apparent molar volume of solute (V^0_ϕ) and apparent molar compressibility of solute (κ^0_ϕ) were obtained from the plots V_ϕ and κ_ϕ as a function of molality and have been utilized in obtaining transfer volumes ($\Delta_{tr}V^0_\phi$) and transfer compressibilities ($\Delta_{tr}\kappa^0_\phi$) of sodium salicylate from water to 0.06 mol·kg^{-1} aqueous solutions of sodium chloride and myo-inositol at different temperatures. The co-sphere overlap model is used to interpret the values of ($\Delta_{tr}V^0_\phi$)and ($\Delta_{tr}\kappa^0_\phi$). The Helper's constant has been obtained. It indicates structure making ability of sodium salicylate in aqueous as well as in 0.06 mol·kg^{-1} aqueous sodium chloride and 0.06 mol·kg^{-1} aqueous myo-inositol solutions. The results obtained have been interpreted in terms of various interactions taking place among solute and solvent molecules.

1. Introduction

Studies of drug action in biological media have always attracted researchers as an outcome of progressive accrual of information from relative techniques of biotech genetics and multidisciplinary sciences [1]. Drug action manifests several thermodynamic changes associated with molecular interactions, whose studies have colossal significance due to the dependence of drug administration, assimilation and response in physiological media. For understanding such molecular interactions (like hydrophobic interaction, hydrophilic interactions and the ionic interactions), drug action has been studied in different physiological media by studying different parameters like volumetric and acoustic properties providing perceptible parameters for the elaboration of (solute-solvent) and (solute-solute) interactions in solution phase [2].

Molecular interactions manifest vital impact of presence of electrolyte and non-electrolyte in physiological media. Their molar volume and compressibility studies could be utilized for taking account of detailed molecular phenomenon occurring therein. Isotonic solution of NaCl (0.06 mol·kg^{-1}) being crucial electrolytic component of extracellular fluids, and myo-inositol a non- electrolyte present in the phosphor inositides of cell membrane and other complex fluids [3], make it ostensible that they may be utilized to investigate drug activity.

Non-steroidal anti-inflammatory drugs (NSAID) comprise a peculiar drug class that groups together those drugs providing non-narcotic, analgesic and antipyretic effects in normal doses. NSAIDs have strong affinity to form ionic and hydrophobic associations with the zwitterionic phospholipids, which are reversible and non-covalent in nature. Sodium salicylate (NaSl)

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(2-Hydroxybenzoic acid sodium salt) being one such NSAID; the study of its volumetric and compressibility properties in variety of aqueous solutions is helpful in interpreting the molecular phenomenon occurring in physiological media [4].

D. Jurivich and co-workers [4] reported that at pH (6.8–7.6) sodium salicylate shows greater molecular interaction between DNA and protein. In further extension to this study, Lichtenberger et al. [5] employed an array of biochemical and biophysical techniques including FTIR, NMR, and Surface Plasmon Resonance (SPR) to propose pH dependence of partition of these drugs. The detailed literature survey reveals that, information is scarce on the volumetric and acoustic properties of sodium salicylate in presence of electrolyte / non-electrolyte media. This fact prompted us to undertake the volumetric and acoustic studies on sodium salicylate in water, aqueous sodium chloride and myo-inositol solutions at different temperatures.

In the present study, the density (ρ) and speed of sound (u) data of sodium salicylate in water, 0.06 mol·kg^{-1} aqueous sodium chloride and 0.06 mol·kg^{-1} aqueous myo-inositol solutions at T = (288.15, 298.15 and 308.15) K within the concentration range (0.01 to 0.1) mol·kg^{-1} are reported. From experimental values, the derived parameters such as the apparent molar volume (V_ϕ) of solute, isentropic compressibility(κ_s) of solution and apparent molar isentropic compressibility (κ_ϕ) of solute have been obtained. The limiting values of apparent molar volume of solute (V_ϕ^0), apparent molar isentropic compressibility of solute(κ_ϕ^0)and apparent molar expansivity (E_ϕ^0) have also been obtained. The solute-solute and solute-solvent interactions occurring in the binary (NaSl + water), ternary (NaSl + water + NaCl) and (NaSl + Water + MI) systems have been discussed with a comment on structure making/breaking tendency of the solute in solutions. The study is vital to understand the nature of biochemical processes and structure effect of bio-fluids in the body system.

2. Experimental

2.1. Chemicals

The chemicals used in the present work, Sodium salicylate (mass fraction purity $\geq$ 0.99) and myo-inositol (mass fraction purity $\geq$ 0.99) were procured from Sigma Aldrich and sodium chloride (mass fraction purity $\geq$ 0.99) was procured from E-Merck, India. All the chemicals were of A.R. grade and were used without further purification. The details are given in Table 1.

Sodium salicylate and myo-inositol were dried in vacuum oven at T = 333.15 K and sodium chloride was dried at T = 423.15 K. All the solutes were kept in vacuum desiccator over anhydrous fused calcium chloride for more than two days before use. All the solutions were prepared in fresh double distilled water on molality basis by using analytical balance (E.Mettler) with an uncertainty in weight up to ±0.1 mg. For aqueous binary system of sodium salicylate, water has been used as solvent and the molality of sodium salicylate has been calculated using 1 kg of water. Whereas, for ternary systems of sodium salicylate, aqueous 0.06 mol·kg^{-1} sodium chloride and aqueous 0.06 mol·kg^{-1} myo-inositol solutions have been used as solvents and the molality has been calculated using 1 kg of aqueous sodium chloride (0.06 mol·kg^{-1}) and 1 kg of aqueous myo-inositol (0.06 mol·kg^{-1}) solutions respectively.

2.2. Methods

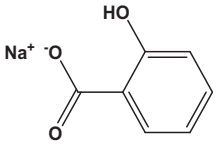
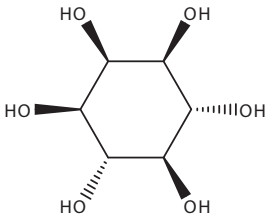
2.2.1. Density measurements

The densities (ρ) of all the binary and ternary solutions were measured at T = (288.15, 298.15, and 308.15) K by using modified Lypkin's bicapillary pycnometers (volume ≈ 28 cm^3). For this purpose pycnometers were immersed in experimental bath. The temperature of the experimental water bath was maintained constant up to ±0.02 K by circulating the thermostatted liquid from Julabo cryostat. The density of pure water at different temperatures was taken from literature [6] and was used to obtain radius of capillary and volume of pycnometer. The pycnometers were calibrated by measuring the density of aqueous solutions of sodium chloride at T = (288.15, 298.15 and 308.15) K within the low concentration range. The density values agreed well with the literature up to ±0.05 kg·m^{-3} [7]. The comparison of experimentally measured densities (ρ) of aqueous 0.06 mol·kg^{-1} NaCl and MI solutions at T = (298.15 and 308.15) K are in good agreement with the corresponding available literature values as presented in Supporting material (Fig. S1) [8–13]. Thereby the combined expanded uncertainty was found to be U_ρ (ρ) = 0.1 kg·m^{-3}. The details have been given elsewhere [14].

2.2.2. Speed of sound measurements

Speeds of sound of all binary and ternary solutions were measured using variable path ultrasonic interferometer (model SI-

Table 1
Provenance and purity of chemical samples.

Chemical Name	Provenance	CAS No.	Mass Fraction Purity[a]	Analysis Method	Structure
Sodium salicylate	Sigma Aldrich	54-21-7	⩾0.99	Titration	
Sodium Chloride	E-Merck	7647-14-5	⩾0.99	LC-MS[b]	Na^+ Cl^-
Myo-inositol	Sigma Aldrich	87-89-8	⩾0.99	GC[c]	

[a] Purity as provided by suppliers.
[b] Liquid chromatography, mass spectrometry.
[c] Gas Chromatography.