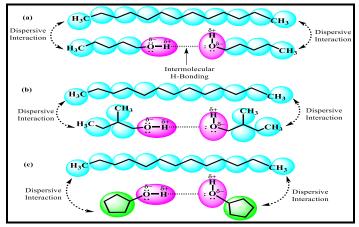
<u>REPORT OF SEED GRANTS/STRENGTHENING RESEARCH GRANT RECEIVED</u> <u>BY PROF. MEENA SHARMA UNDER RUSA 2.0</u>

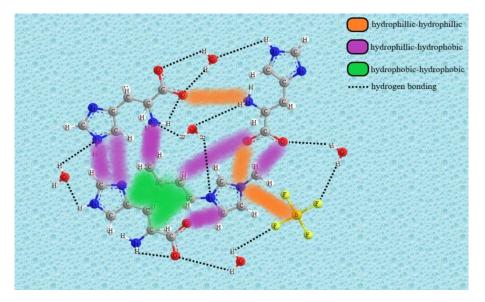
The seed money received under RUSA 2.0 has been utilized for research work proposed in the project proposal. The salient features of the work done are discussed below:

1. Experimental data of density (ρ), viscosity (η) and speed of sound (u) at seven temperatures from (293.15-323.15) K with an interval of 5K has been determined for the binary systems: Tridecane + 1-pentanol, Tridecane + 2-methyl -1-butanol and Tridecane + cyclopentanol over entire range of composition. Excess parameters such as excess molar volume (V_m^E), deviations in viscosity ($\Delta\eta$), excess isentropic compressibility (κ_s^E) and excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) have been computed and correlated using Redlich Kister polynomial equation. The weakening of intermolecular hydrogen bonding existing among alcohols due to prevailing dispersive interactions among non-polar regions of binary system have been interpreted in terms of various derived thermodynamic parameters. The V_m^E values have been found to be positive while $\Delta\eta$ values have been found to be negative for studied binary systems at various temperatures. The positive κ_s^E values for all the three binary system reveals the extent of compactness of mixtures, but these values are found to be negative after 0.5 mole fraction (x_1) for Tridecane + Cyclopentanol system. Such investigations are essential for design and better performance of hydrocarbon fuels.



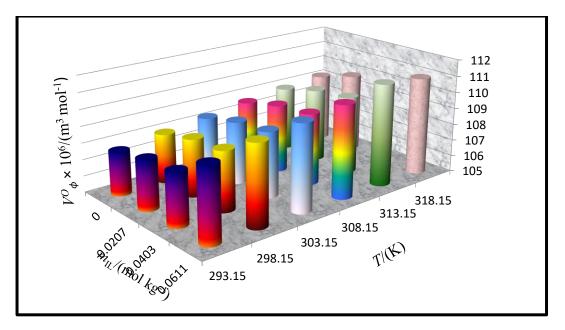
Journal of Chemical & Engineering Data, 67.5 (2022) 1054-1069

2. Experimentally density (ρ), viscosity (η) and speed of sound (u), have been measured for L-Histidine in aqueous ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ([C₄mim][BF₄]) solutions at different temperatures ranging (293.15-318.15) K. Using examined data various volumetric, viscometric and compressibility parameters, i.e. apparent molar properties ($V_{\phi}, K_{\phi,S}$), limiting apparent molar properties ($V_{\phi}^{o}, K^{o}_{\phi,S}$), transfer properties ($V_{\phi,tr}^{o}, K_{\phi,S,tr}^{o}, B_{tr}$) and viscosity coefficients A and B have been computed, which are used to investigate the precious information about the complicated phenomenon undergoing between ionic liquid $[C_4mim][BF_4]$ and the head/side chain cluster of amino acid. Based on co-sphere overlap model variety of intermolecular interactions prevailing in the ternary solutions have been enlightened along with the structure making/breaking nature of solute using Hepler's constant and temperature derivative of *B*-coefficients (*dB/dT*).



Journal of molecular liquids, 303 (2020) 112596

3. The effect of ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ([C₄mim][BF₄]) (IL) on the thermophysical performance of amino acid (aa) has been examined by using viscometric, volumetric and acoustic approach. In such approach viscosity, density and speed of sound has been quantified experimentally for L-leucine in aqueous IL (0.0207, 0.0403, 0.0611) mol kg⁻¹ solution at various temperatures (293.15-318.15) K to appraise the different parameters i.e. apparent molar properties ($V_{\phi}, K_{\phi,s}$), limiting apparent molar properties ($V^{o}{}_{\phi}, K^{o}{}_{\phi,s}$), limiting apparent molar transfer properties $(V^{o}_{\phi,tr}, K^{o}_{\phi,s,tr}, B_{tr})$, viscosity coefficients A and B and hydration number (n_H) . The resulting data of evaluated parameters are resolved on the basis of co-sphere overlap model, which explain the existence of different intermolecular interactions in the system and positive transfer values signify the dominance of ionichydrophilic interactions. Moreover the structure making/breaking character of solute is deciphered by the temperature derivative of viscosity B-coefficients (dB/dT) and Hepler's constant.



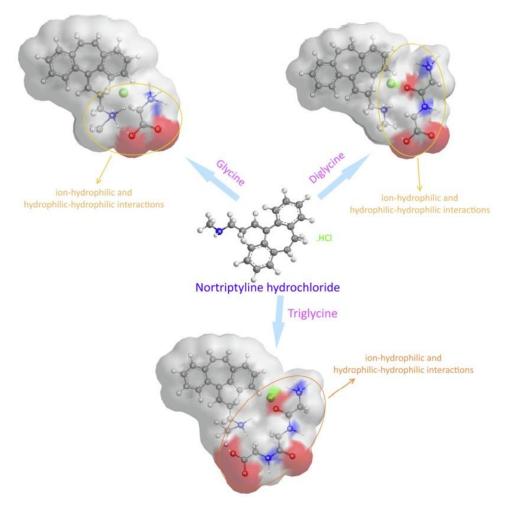
Journal of chemical thermodynamics, 2106696 (2021)

4. From the measurements of density, (ρ) and speed of sound, (u), the intermolecular interactions of D-maltose monohydrate and D-lactose monohydrate with trisodium citrate (TSC) have been explored in aqueous medium at temperatures, T = (293.15-313.15) K, pressure p = 0.1 MPa. From the experimental density measurements, apparent molar volume (V_{ϕ}) , limiting apparent molar volume (V_{ϕ}) and limiting apparent molar volume of transfer $(V_{\phi,tr})$ have been determined for various solutions of maltose and lactose in aqueous TSC. In addition, using experimental speed of sound data, apparent molar isentropic compressibility $(K_{\phi,s})$, limiting apparent molar isentropic compressibility $(K_{\phi,s})$, have been calculated. Further, apparent molar expansibility (E^o_{ϕ}) , Hepler's constant values $\left(\frac{\partial E^o_{\phi}}{\partial T}\right)_p$ and hydration number $(n_{\rm H})$ have been assessed to contribute the interpretations received from the acoustic and analysis. The assessed outcomes were construed in terms of diverse intermolecular interactions present in the ternary systems (saccharides+ water + TSC) through a co-sphere overlap model. From the Hepler's constant structure breaking nature of the solute have been confirmed.

Chemical Thermodynamics and Thermal Analysis, 6 (2022) 100051.

5. From the density (q), speed of sound (u) and viscosity (g) measurements, the interactions of glycine, glycylglycine and glycylglycylglycine with antidepressant drug, nortriptyline hydrochloride have been investigated in aqueous medium at temperatures, T = (293.15-313.15) K and experimental pressure p = 0.1 MPa. From the experimental

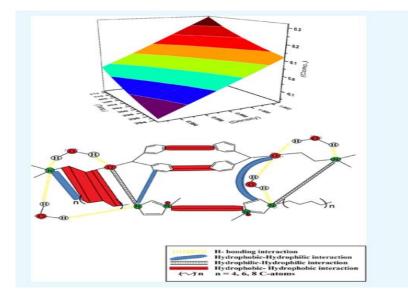
density measurements, apparent molar volume, limiting apparent molar volume (Vo U) and partial molar volumes of transfer, have been determined for various solutions of glycine, glycylglycine and glycylglycylglycine in aqueous nortriptyline hydrochloride. In addition, using speed of sound data, apparent molar isentropic compression, limiting apparent molar isentropic compression and partial molar isentropic compression of transfer have been calculated. Pair and triplet interaction coefficients are also determined from values using McMillan-Mayer theory. Further, apparent molar expansibility and Hepler's constant values have been evaluated to assist the interpretations earned from the volumetric and acoustic analysis. The viscosity coefficients (d*B*/dT) have been determined from viscosity data. The results were interpreted in terms of different kinds of intermolecular interactions present in the ternary systems (amino acid/pep tides + water + nortriptyline hydrochloride) through a co-sphere overlap model. The Hepler's constant and temperature derivative of *B*-coefficients (d*B*/dT) confirms the structure breaking nature of the solute.



Journal of Molecular Liquid, 354 (2022) 118760

6. In the present work, we attempt to study the interaction between the DPH drug and three imidazolium ionic liquids in aqueous medium via a volumetric and acoustic approach. The apparent partial molar volume $(V\phi)$ and the partial molar isentropic

compressibility $(K\phi)$ were evaluated from experimental density and acoustic data, respectively. It was found that both these quantities showed an enhanced trend with increasing ionic liquid concentration in all of the ternary systems. Moreover, the interactions between DPH and the ionic liquids were strengthened with increasing ionic liquid concentrations. Also, these interactions increase with the increase in size of the alkyl chain length of the ionic liquids. There occur strong solute- solvent interactions in the ternary system, which is confirmed by the derived partial molar properties of transfer. The Helper's constant $(\partial E \phi \circ / \partial T)P$ calculation finally concludes DPH as a structure maker, and its structure-making behavior increases with increasing ionic liquid concentrations. From the UV data, a general increase in the intensity of the absorption maxima with the increase in ionic liquid concentrations and with the addition of a small amount of DPH is observed. Further, a hypsochromic shift is observed with the addition of a small amount of DPH in aqueous ionic liquid solution, which indicates that the solute- solvent interaction is prevailing in the ternary system. Finally, the present results confirm the presence of strong ionic- hydrophilic and hydrophilic-hydrophilic interactions between the DPH molecules and the ionic liquids, and the comprehensive behavior of these interactions in getting more stronger with the increase in size of the alkyl chain length of the ionic liquids.



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STRENGTHENING OF RESEARCH AND SEED GRANT 2019-2020

S. No	Name of Faculty	Grant Received	Utilized	Unspent
1.	Prof. Meena Sharma	4,00,000/-	3,99,924/-	76/-
2.	Prof. S.K Pandey	3,95,000/-	3,94,592/-	408/-
3.	Prof. K.K Kapoor	4,25,000/-	3,93,421/-	31,579/-
4.	Prof. H.N Sheikh	4,50,000/-	4,49,849/-	151/-
5.	Prof. Satya Paul	4,20,000/-	3,98,713/-	21,287/-
6	Prof. D.S Sambyal	4,00,000/-	3,99,256/-	744/-
7	Dr. Monika Gupta	1,00,000/-	99682/-	318/-
8	Dr. Ashwani Kumar	1,00,000/-	99,699/-	301/-
9	Prof. R.K Bamezai	4,10,000/-	99,071/-	3,10,929/-
10	Dr. G.D Bajju	4,50,000/-	4,34,405/-	15,595/-

Prof. Kamal K. Kapoor Head of the Department

Joint Registrar (Finance) University of Jammu. Journal of Molecular Liquids 303 (2020) 112596



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Molecular interactions of L-Histidine in aqueous ionic liquid [C₄mim] [BF₄] solution at different temperatures: Volumetric, acoustic and viscometric approach



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ABSTRACT

Experimentally measured density (ρ), viscosity (η) and speed of sound (α) for L-Histidine in aqueous ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ($[C_4mim][BF_4]$) solutions at different temperatures ranging (293.15–318.15) K has been used to determine various volumetric, viscometric and compressibility parameters, i.e. apparent molar properties ($V_{\alpha_1}K_{\alpha_1+}$), limiting apparent molar properties ($V^{\alpha_{\alpha_2}}K^{\alpha_{\alpha_3}}$), transfer properties ($V^{\alpha_{\alpha_3}}, K^{\alpha_{\alpha_3}}, B_{\alpha_3}$), hydration number (n_{α_1}). Viscosity coefficients A and B have been computed to investigate the precious information about the complicated phenomenon undergoing between ionic liquid [C_4mim][BF₄] and the head/side chain cluster of amino acid. Based on co-sphere overlap model variety of intermolecular interactions prevailing in the ternary solutions and using Hepler's constant and temperature derivative of Bcoefficients (dB/dT) the structure making/breaking nature of solute have been investigated.

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1. Introduction

The importance of thermophysical and thermodynamic studies is to interpret structure and molecular interactions with the help of collected and calculated data of compounds and their combinations with other solutes/solvents [1–4]. Proteins are the structural materials in all living beings and involved in various biological reactions. The obligatory task of proteins in all the biological processes can only be understood by the sensitivity of its adjoining environment, Modification in the chemical and biological behavior, inter-ionic interactions and stability of proteins on varying its surrounding environment formulates to study the proteins behavior in the presence of different solvents. Amino acids and small peptides, the structure block of proteins are considered as the model compounds to study the effect of additives (electrolytes, surfactants, drugs etc.) on proteins [5–8] because it is difficult to directly evaluate the physicochemical properties and interactions of proteins due to their complex configuration and conformation.

We lack in our knowledge about interactions of the solvent predominantly water, the plenteously used biological solvent and its complexity

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which become more complicated in the presence of various solutes (amino acids, drugs, peptides, inorganic and organic salts etc.). In the recent past, it has been found that the physicochemical studies of amino acids [4,9-11] or small peptides [12-14] in water are of significant importance as these are corridor for fundamental understanding of the various interactions as well as structural transformations of natural building blocks, amino acids/proteins in diverse and complicated biological processes. Appraising their applications, amino acids/peptides with different additives have been examined numerously. These days, the frequently used additives are ionic liquids whose unique and fascinating properties, make them available to replace a broad range of volatile organic compounds. They have also been engaged in altering the statistical, structural, bio-catalytic and enzymatic activity of proteins [4,9,11,15]. Numbers of branches are involved to study the ionic and molecular interactions of these ionic liquids with various biomolecules which help to investigate and realize the unusual features of solution chemistry. Weak molecular interactions (like solute-solute and solute-solvent interactions) existing in the solutions are complicated and difficult to understand but hold the factual explanation for the complex nature of diverse properties of the solute in solutions and more particularly to comprehend the molecular interaction of ionic liguid + amino acids in an aqueous solvent. Zhao et al. [2] studied the effect of three ionic liquids [C2mim]Br, [C4mim]Br and [C8mim]Br on the

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Study on molecular interactions of L-leucine in aqueous ionic liquid (1butyl-3-methylimidazolium tetrafluoroborate) [C₄mim][BF₄] solution using density, speed of sound and viscosity measurements at various temperatures



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ABSTRACT

The effect of ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ($|[C_qmim]|[BF_q]$) (IL) on the thermophysical performance of amino acid (aa) has been examined by using viscometric, volumetric and acoustic approach. In such approach viscosity, density and speed of sound has been quantified experimentally for L-leucine in aqueous IL (0.0207, 0.0403, 0.0611) mol kg⁻¹ solution at various temperatures (293.15–318.15) K to appraise the different parameters i.e. apparent molar properties ($V_{\Phi,K}, K_{\Phi,k}$), limiting apparent molar properties ($V_{\Phi,K}^{\alpha}, K_{\Phi,k}^{\alpha}$), limiting apparent molar transfer properties ($V_{\Phi,K}^{\alpha}, K_{\Phi,k}^{\alpha}$), limiting apparent molar properties ($V_{\Phi,K}^{\alpha}, K_{\Phi,k}^{\alpha}$), limiting apparent molar transfer properties ($V_{\Phi,K}^{\alpha}, K_{\Phi,k,R}^{\alpha}$), viscosity coefficients A and B and hydration number (n_{H}). The resulting data of evaluated parameters are resolved on the basis of co-sphere overlap model, which explain the existence of different intermolecular interactions in the system and positive transfer values signify the dominance of ionic-hydrophilic interactions. Moreover the structure making/breaking character of solute is deciphered by the temperature derivative of viscosity B-coefficients (dR/dT) and Hepler's constant.

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1. Introduction

The thermodynamic and thermophysical studies of compounds in combination with various solutes/solvents made available the accurate information to design, develop and improve the novel purification and separation methods for biomolecules in the solution [1-4]. Among the biomolecules, proteins are majorly involved in all life forms structurally and functionally to perform countless biological reactions. The occurrence of non-covalent interactions (hydrophobic interactions, electrostatic, and hydrogen-bonding) in their native form is responsible for their stability. This stability gets disturbed, i.e. enzymatic activity, solubility, chemical behavior, and hydration get affected when the presence of solute and solute-solvent interactions modify the structure of water, the prolifically utilized biological solvent. Consequently, it becomes essential to find out the functionality and state of proteins in various mediums to understand their biological and chemical behavior in a better way. To elucidate these phenomena, the model low molecular mass component of proteins (amino acids/peptides) has been scrutinized as the straight thermophysical study of complex threedimensional protein is not viable [5–9]. By considering their applications, the physicochemical studies of these model components i.e. amino acid [3–7,9–10]/peptides [11–13] in water with various additives (drugs, electrolytes, inorganic, organic salts, etc.) have attracted the attention of many researchers in recent times, as this provides a corridor to comprehend the structural transformation in composite biological processes as well as various molecular interactions, where side chains of peptide and amino acid contribute towards the type and magnitude of interactions.

The repeatedly utilized additives at present are room temperature ionic liquids (ILs): the greener solvents whose mesmerizing and matchless properties like better protein stability, high selectivity, high conversion rates along in better recyclability and recoverability replacing a wide array of volatile organic compounds [14]. To explore the effect of thermodynamic variables (temperature and pressure) and unusual properties of solution chemistry, the number of branches are engrossed in analyzing the physical immutability, molecular interactions (solute-solvent, solute-solute) of biomolecules with various ILs which are significant to perceive the stability of proteins in numerous physiological and biochemical procedures in a cell. It is hard to get the existing weak intermolecular interactions in the ternary solutions however they embrace the accurate enlightenment about the complex phenom-



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Effect of trisodium citrate dihydrate on thermophysical properties of saccharides in aqueous media at different temperatures: Volumetric and acoustic properties



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ARTICLE INFO

Keywords: Spoed of sound Density Apparent mólar volume Hepler's constant Apparent mólar compressibility DSA

ABSTRACT

From the measurements of density, (ρ) and speed of sound, (μ), the intermolecular interactions of D-maltose monohydrate and D-lactose monohydrate with trisodium citrate (TSC) have been explored in aqueous medium at temperatures, T = (293.15-313.15) K, pressure p = 0.1 MPa. From the experimental density measurements, apparent molar volume (V_{Φ}), limiting apparent molar volume ($V_{\Phi_{\Phi}}$) and limiting apparent molar volume of transfer ($V_{\Phi_{\Phi,\mu}}$) have been determined for various solutions of maltose and lactose in aqueous TSC. In addition, using experimental speed of sound data, apparent molar isentropic compressibility ($K_{\Phi_{\mu,\mu}}$), limiting apparent molar isentropic compressibility ($K_{\Phi,\mu}^*$) and partial molar isentropic compression of transfer ($K_{\Phi_{\mu,\mu}^*}^*$) have been calculated. Further, apparent molar expansibility ($E_{\Phi_{\Phi}}^*$), Hepler's constant values($\frac{\delta E_{\Phi}}{\delta T}$) and hydration number ($n_{\mu,\mu}$)have been assessed to contribute the interpretations received from the acoustic and analysis. The assessed outcomes were construed in terms of diverse intermolecular interactions present in the ternary systems (saccharides + water + TSC) through a co-sphere overlap model. From the Hepler's constant structure breaking nature of the solute have been confirmed.

1. Introduction

The thermodynamic and thermophysical studies of compounds in combination with various solutes/solvents made available the accurate information to design, develop and improve the novel purification and separation methods for biomolecules in the solution [1-4]. Thermodynamic properties of solutions, like acoustical properties and volumetric properties provides valued statistics concerning the various intermolecular interactions(ion-dipole, dipole-dipole, and H-bonding, etc), which has a prodigious importance in physical chemistry, environmental chemistry, surface chemistry, biological chemistry and geochemistry. Saccharides are known as characteristic nonelectrolytes bearing numerous hydroxyl groups and hence extensive range of forms, which shows its great versatility in biological activities such as metabolic recognition, assistance in stabilizing the inherent configurations of globular proteins [5-8] and lipid bilayers during dehydration [9-11]. The conformation of the hydroxyl groups [12,13] and its number has controlled the hydrational behavior of carbohydrates. Thus, the hydration properties of saccharides is a significant trait in defining their functional and structural properties [10,13-16]. In food industry and biological industry, thermodynamic studies of saccharides in aqueous mixed solutions have a critical role. The carbohydrate units in a cell are the receptors of functionalised compounds like drugs, enzymes etc. Soluble carbohydrates (fructose, sucrose and glucose) with additives like salts, glycerol, ethanol in aqueous binary and ternary solutions act as an appropriate medium for freezing fruits. In yeast, brine shrimps, mushroom and fungi, the intracellular a,a-trehalose subsidizes during its vitrification to their existence capabilities in contradiction of spartan situations like desiccation and freezing. In aqueous solution, the labile biomolecules have been stabilized by saccharides through the blend of its specific and kinetic effects [17,18].

With the addition of salts in aqueous carbohydrate systems, their properties like crystallization rate, viscosity, glass transition temperature and water sorption have been modified. The K⁺ and Na⁺ ions are primarily accountable for osmotic pressure of biofluids and the prominent alteration in the arrangement of intracellular and extracellular fluids in sap fluids in plants and animals [19-21]. In aqueous solutions of metals ions, the interaction of saccharide residues of biological compounds with metal ions have been improved. Despite the feeble metalsaccharide complexes formed, their communications are choosy. Still, stabilities of the complexes formed, their preferences in binding, stereochemical and structural features are not finely tacit [22-25]. Aqueous

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Volumetric, acoustic and viscometric studies of solute-solute and solutesolvent interactions of glycine and its peptides in aqueous solutions of an antidepressant drug at different temperatures



IOUIDS

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ABSTRACT

From the density (ρ), speed of sound (u) and viscosity (η) measurements, the interactions of glycine, glycylglycine and glycylglycylglycine with antidepressant drug, nortriptyline hydrochloride have been investigated in aqueous medium at temperatures, T = (293.15-313.15) K and experimental pressure p = 0.1 MPa. From the experimental density measurements, apparent molar volume (V₀), limiting apparent molar volume (V^{*}_{Φ}) and partial molar volumes of transfer $(V^{*}_{\Phi,r})$ have been determined for various solutions of glycine, glycylglycine and glycylglycylglycine in aqueous nortriptyline hydrochloride. In addition, using speed of sound data, apparent molar isentropic compression $(K_{s,\Phi})$, limiting apparent molar isentropic compression $(K^{*}_{s,\Phi})$ and partial molar isentropic compression of transfer $(K^{*}_{s,\Phi,tr})$ have been calculated. Pair and triplet interaction coefficients are also determined from V° our values using McMillan-Mayer theory. Further, apparent molar expansibility (E°_{ϕ}) and Hepler's constant values $\left(\frac{dt_0}{dt}\right)_n$ have been evaluated to assist the interpretations earned from the volumetric and acoustic analysis. The viscosity coefficients A and B, viscosity B-coefficient of transfer (Brr) and temperature derivative of B-coefficients (dB/dT) have been determined from viscosity data. The results were interpreted in terms of different kinds of intermolecular interactions present in the ternary systems (amino acid/pep tides + water + nortriptyline hydrochloride) through a cosphere overlap model. The Hepler's constant and temperature derivative of B-coefficients (dB/dT) confirms the structure breaking nature of the solute. © 2022 Elsevier B.V. All rights reserved.

1. Introduction

Life has been started with innovative and constant chemical reaction series which elevate the non-living material to higher levels. We all know, atoms accumulated to compounds, which then transformed into complex ones and lastly, the utmost complex form of them transformed into ordered living cells. In the modern era, a drug discovery and drug-protein interactions play a vital role in all the biological and metabolic pathways occur within the living body [1–3]. The drug's interaction has been transpired mainly during its formulation, mixing ingredients, storage and its physical or chemical activity outside the body. The main area of drug discovery involves the recognition of new molecular target proteins and their pharmacological action in medical needs [4,5]. In general the biochemical processes ensue in aqueous media. The presence of water as a major component in bio systems triggers the

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hydrophobic forces, the prime factor in stabilizing the structure and properties of proteins [6,7]. Several experimental quantifications, specifically the physico-chemical measurements and thermodynamic measurements has been done by manifold researchers to comprehend the drug activities such as movement through the bloodstream, its spreading, binding with receptor, anticipated action and their molecular interactions with biological molecules in aqueous and non-aqueous solutions. The drugsolvent interactions in the ternary systems get reformed with temperature and in the presence of co-solutes (third component) such as polymer, salt, osmolytes, carbohydrate, amino acid, surfactant, alcohol, peptide, etc. Usually, in drug molecules both the hydrophobic and hydrophilic groups are clutched. Thus, they display numerous specific interactions and non-specific interactions in aqueous medium. Volumetric, acoustic and viscometric measurements are the important tool in illuminating these types of interactions (ion-dipole, dipole-dipole, and H-bonding, etc.). It is rather challenging for the researchers to get the feasible facts and thermophysical data for the proteins in composite aqueous

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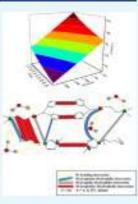


Molecular Interactions of Diphenhydramine-hydrochloride with Some Imidazolium-Based Ionic Liquids in Aqueous Media at T = 293.15–313.15 K: Volumetric, Acoustic, and UV Absorption Studies

Jeetinder Singh, Manjeet Singh, Samriti Sharma, Shubham Sharma, and Meena Sharma*

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diphenhydramine-hydrochloride (DPH) with three imidazolium-based ionic liquids (ILs) (1-butyl-3methylimidazolium chloride, $[C_4mim][Cl]$, 1-hexyl-3-methylimidazolium chloride1, $[C_6mim][Cl]$, and 1-methyl-3-octylimidazolium chloride, $[C_8mim][Cl]$) have been investigated in aqueous medium at T =293.15–313.15 K and experimental pressure p = 0.1 MPa. From the density calculations, the apparent molar volume (V_{ϕ}) and the apparent partial molar volumes of transfer ($\Delta_i V_{\phi}^n$) have been determined for various solutions of DPH in aqueous solutions of different ILs. In addition, from the speed-of-sound data, the apparent molar isentropic compressibility (K_{ϕ}), apparent partial molar isentropic compressibility (K_{ϕ}^n), and apparent partial molar isentropic compressibility of transfer ($\Delta_i K_{\phi}^n$) have been calculated. The pair and triplet interaction coefficients are derived from apparent partial molar volumes of transfer. For the present mixtures, the absorption spectra have been also recorded using a UV-visible spectrophotometer. Using Hepler's constant, the structure-making nature of the solute has been confirmed. All these calculated parameters provide detailed insights into various physicochemical



interactions prevailing in the ternary system and confirm the presence of a strong attractive interaction between DPH and ILs.

1. INTRODUCTION

Ionic liquids have emerged as powerful and promising green solvents in various industrial and academic areas.1 In general, ionic liquids are a class of organic salts composed of bulky asymmetric organic cations (e.g., imidazolium, pyridine, etc.) and organic or inorganic anions (e.g., halides) that are liquids below 373 K.2 The attractiveness of these comforting solvents has been attributed to their unusually unique properties such as very small vapor pressure, a wide liquid range, high thermal stability, and excellent solvent power for organic and inorganic compounds.^{3,4} In particular, the low vapor pressure ascribed to their ionic inherent characteristics along with their good thermal stability make them "green" alternatives to conventional hazardous organic solvents.⁵ Due to their structural modification activities, ILs are termed as "designer" or "task-specific" solvents. Studies have shown that ionic liquids have efficient applications in the fields of biomass conversion,", biotransformation, electrochemistry,9 liquid crystal development,10 chemical synthesis and catalysis,11,12 biotechnology, and many other fields like medicine and the pharmaceutical industry.13,14 Comprehensive studies of ILs can serve to better understand the functional mechanisms of important biomolecules such as amino acids, histidine, etc., which contain imidazole side chains and play a vital role in the structure and binding functions of hemoglobin.

The emerging progress in biotechnology and genetics in the recent times has widened the scientific interest in exploring the action of drugs in biological media.¹⁴ The drug-water molecular interactions and their temperature dependence play a pivotal role in understanding the drug action.¹⁵ Investigation of thermodynamic, volumetric, and acoustical properties is an important tool in determining the intermolecular interactions occurring in electrolyte solutions. Further, studies on the volumetric and acoustic properties of aqueous ionic liquid—drug solutions provide crucial information on the interactions, solvation, and association behavior of ions in such solutions.^{16–20} Abundant studies on the thermodynamics, viscometry, phase equilibria, and surface phenomenon of ILs in pure solution and as mixtures especially with water have been used as the basis for several reactions.^{21–24}

In the present work, we have studied the volumetric and acoustic properties of DPH in aqueous mixtures of [C₄mim]-[Cl], [C_nmim][Cl], and [C₈mim][Cl]. The focus of our work is to present some new thermodynamic properties of the mentioned ternary systems. In the current study, DPH has been chosen as a drug candidate because of its water-soluble nature and its significant medical applications. In medicine, this drug is used to treat insomnia, symptoms of common cold, tremor in Parkinsonism, extrapyramidal symptoms, and

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