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Effect of N-acetylglycine on volumetric and acoustic behaviour of aqueous tetrabutylammonium iodide solutions at different temperatures

Suresh Kumar Sharma [a,*], Gurpreet Singh [a,c], Harsh Kumar [b], Ramesh Kataria [c]

[a] Department of Chemistry, D. A. V. College, Abohar 152116, India
[b] Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144011, India
[c] Department of Chemistry, Panjab University, Chandigarh 160014, India

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ABSTRACT

In this work, the experimental densities and ultrasonic speeds of N-acetylglycine in (0.01, 0.02, 0.03 and 0.04) mol·kg^{-1} aqueous tetrabutylammonium iodide (TBAI) solutions have been reported at temperatures (288.15, 293.15, 298.15, 303.15 and 308.15) K and at pressures 101 kPa. The different parameters such as apparent molar volume, limiting apparent molar volume, transfer volume, partial molar expansibility have been derived from density data. Experimental values of ultrasonic speeds were used to estimate coefficient of isentropic compression, apparent molar isentropic compression, limiting apparent molar isentropic compression and its transfer value. The pair and triplet interaction coefficients have also been calculated from transfer parameters. All these parameters offer a convenient method to study the intermolecular interactions between the various components of the ternary mixtures. The interactions increase with increase in the concentration of N-acetylglycine in aqueous TBAI solutions. The variation of these parameters with concentration and temperature clearly suggests the role of $(C_4H_9)_4N^+$ on the solute–solvent interactions in aqueous medium.

1. Introduction

Salt solutions have large effects on the structure and properties of proteins including their solubility, denaturation, dissociation into subunits, and the activity of enzymes [1–3]. Proteins are complex molecules, and their behaviour in solutions is governed by a combination of many specific interactions. One approach that reduces the degree of complexity and requires less complex measurement techniques is to study the interactions in systems containing smaller biomolecules such amino acids and peptides. Importance of studying the smaller biomolecules having low molecular weight lies in the fact that one can systematically alter the structure and therefore contribution of side chain groups of amino acid and peptide can be seen easily. It would be interesting to see the chances in the group contributions of limiting partial molar volume upon transferring the side chains from the α-amino acids to other amino acid derivatives *e.g.* N-acetylamino acids. The N-acetylamino acids constitute a class of compounds in which the electrostriction effect would not be present to perturb the partial molar volume contribution of the peptide or alkyl groups. In proteins or polypeptides the majority of the alkyl side chains are situated in the environment of dipolar —CONH groups. Thus, the partial molar volume contribution of alkyl side chains in the N-acetylamino acids may represent a value close to that in polypeptides or proteins.

Some studies [4,5] have revealed that the presence of an electrolyte drastically affects the behaviour of amino acids in solutions, and this fact can be used for their separation and purification. Thermodynamic properties of amino acids in aqueous electrolyte solutions thus provide valuable information about solute–solvent and solute–solute interactions. Hence there has been a number of works [6–14] revealing the effect of electrolyte solutions on amino acids. Salts such as tetraalkylammonium halides can give a better insight into the effect of electrostatic and hydrophobic interactions on the stability of proteins as these salts are known to influence macromolecular conformations by weakening attraction or repulsion of inter and intra charge-transfer interactions and by affecting hydrophobic interactions through the side chain of the alkyl groups. Tetraalkylammonium salts are bulky in nature and are known to orientate water molecules around them depending on their alkyl chain [15,16]. They do not interact electrostatically with water molecules being hydrophobic in nature. In order to avoid

* Corresponding author.
E-mail address: suresh30091978@gmail.com (S.K. Sharma).

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contact with water, R_4N^+ cation sits in the cavities created by the tetrahedrally arranged water molecules resulting into the tighter packing. The R_4N^+ cations are strong structure-maker because of their large size, weak charge and their inability to break down tetrahedral structure of water.

A number of workers [17–25] have studied the volumetric, viscometric and acoustic properties of amino acids in aqueous tetra-n-alkylammonium salts while such studies on substituted amino acids in aqueous tetraalkylammonium salts are rare. In order to understand the interactions between N-acetylamino acids and tetraalkylammonium salts, we [26] have very recently reported the densities and ultrasonic speeds of N-acetylglycine in aqueous solutions of tetraethylammonium iodide (TEAI) at different temperatures. These investigations revealed that the extent of solute–solvent interactions increases with the increase in concentration of TEAI. The presence of TEAI facilitates the solute-co-solute interactions in N-acetylglycine at lower temperature while ion–hydrophobic and hydrophobic–hydrophobic interactions are predominating at higher temperatures.

In continuation of recent work on these mixtures [26], we now report the densities and ultrasonic speeds of N-acetylglycine in aqueous tetrabutylammonium iodide (TBAI) solutions at temperatures (288.15, 293.15, 298.15, 303.15 and 308.15) K. The temperatures are chosen because much more relevance and significance can be achieved by studying compounds of biological importance at different temperatures. As per our knowledge, no data on thermodynamic studies of N-acetylglycine with aqueous TBAI have been reported so far.

2. Experimental

2.1. Materials

N-acetylglycine of high purity (mass fraction $\geqslant 0.99$) used in the present study was purchased from SD Fine Chem. Ltd., India. Reagent grade N-acetylglycine was recrystallized twice in (ethanol + water) mixtures, dried at $T = 383.15$ K. Tetrabutylammonium iodide (TBAI) (mass fraction > 0.98) were procured from Acros Organics, New Jersey, USA and purified by recrystallization to ensure maximum purity and dried in vacuum. Both the chemicals were kept over P_2O_5 in a vacuum desiccator for minimum of 48 h prior to use. The specifications and structures of the chemicals used in this study are given in table 1.

2.2. Methods

The stock solutions (0.01, 0.02, 0.03 and 0.04) mol·kg^{-1} of TBAI were prepared in triply distiled water and were used as solvents for the preparation of N-acetylglycine solutions of different molal concentrations ranging from (0 to 0.2) mol·kg^{-1}. All the solutions were weighed by an A&D company, limited electronic balance (Japan, Model GR-202) with a precision of ±0.01 mg. The standard uncertainty in molality as per stated purities is $u_r(m) = 0.01$ (*i.e.* 1% relative uncertainty). The specific electrical conductivity of triply distiled water used was less than 10^{-6} S·cm^{-1}. The solutions were prepared with utmost care and stored in special airtight bottles to avoid moisture contamination and evaporation. N-acetylglycine was considered as the solute while the additive TBAI was considered as co-solute.

The densities (ρ) and ultrasonic speeds (c) of the sample solutions were measured simultaneously and automatically, using an Anton Paar DSA 5000 M densimeter (oscillating U-tube density and speed of sound analyser). The ultrasonic speed is measured using a propagation time technique. The sample is sandwiched between two piezoelectric ultrasound transducers. One transducer emits sound waves through the sample-filled cavity at a frequency of approximately 3 MHz; the second transducer receives these waves. Thus, the ultrasonic speed (c) is obtained by dividing the known distance between transmitter and receiver by the measured propagation time of the sound wave [27]. A density check or an air/water adjustment was performed at 20 °C with triply distiled, degassed water, and with dry air at experimental pressure. Before each series of measurements, the densimeter was calibrated with triple distiled and degassed water, cyclopentane, propanol and benzene at each measuring temperature through a special adjustment procedure driven by built-in software. Both density and ultrasonic speed are extremely sensitive to temperature, so it was controlled to $\pm 1 \cdot 10^{-2}$ K by built-in Peltier device. The sensitivity of the instrument corresponds to a precision in density and ultrasonic speed measurements of $\pm 1 \cdot 10^{-3}$ kg·m^{-3} and $\pm 1 \cdot 10^{-2}$ m·s^{-1}, respectively. The standard uncertainty of the density and ultrasonic speed estimates was found to be within ±1 kg·m^{-3} and $\pm 5 \cdot 10^{-1}$ m·s^{-1}, respectively.

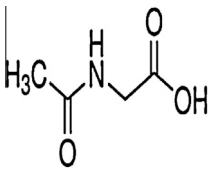
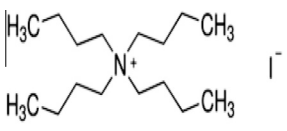
3. Results and discussion

3.1. Analysis of density and ultrasonic speed results

The experimental values of densities and ultrasonic speeds obtained for N-acetylglycine in (0.01, 0.02, 0.03 and 0.04) mol·kg^{-1} TBAI solutions at temperatures (288.15, 293.15, 298.15, 303.15 and 308.15) K are given in table 2. The experimental values of densities and ultrasonic speeds were analysed by least square fitting using following equations:

$$\rho = a + bm + cm^2, \quad (1)$$

TABLE 1
Specification of chemical samples.

Chemical name	Provenance	[a] Mass fraction purity	Purification method	Structure
N-acetyl glycine	SD Fine Chem. Ltd., India CAS No. 543-24-8	>0.99	Recrystallization	
Tetrabutylammonium iodide	Acros Organics, New Jersey, USA CAS No. 311-28-4	>0.98[b]0.998	Recrystallization	

[a] As declared by supplier.
[b] Mass fraction purity as per certificate of analysis provided by manufacturer.