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Solvation behavior of glycine and glycyl dipeptide in aqueous 1-butyl-3-methylimidazolium bromide ionic liquid solutions at different temperatures

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ABSTRACT

Densities and speeds of sound of glycine and glycyl dipeptide (glycylglycine) in aqueous 1-butyl-3 methylimidazolium bromide, [C_4mim][Br] solutions have been measured at $T = (288.15, 298.15$ and $308.15)$ K. From the experimental data of density and speed of sound, the apparent molar volumes (V_ϕ), apparent molar volumes at infinite dilution (V_ϕ^0), apparent molar isentropic compression ($K_{\phi,s}$) and apparent molar isentropic compression at infinite dilution ($K_{\phi,S}^0$) have also been determined. Further, the partial molar volumes of transfer ($\Delta_{tr}V_\phi^0$) and partial molar isentropic compression of transfer ($\Delta_{tr}K_{\phi,S}^0$) of glycine and glycyl dipeptide from water to aqueous [C_4mim][Br] solutions were calculated to enlighten the interactions such as solute–solute, solute–solvent and solvent–solvent present in these solutions. The apparent molar expansivity (E_ϕ^0), Hepler's constant values $(\frac{\partial E_\phi^0}{\partial T})_P$, thermal expansion coefficient (α) and hydration number (n_H) have been evaluated to assist the interpretations earned from the volumetric and acoustic analysis. The Hepler's constant values were found negative for glycine and glycyl dipeptide at all concentrations of ionic liquid except at lower concentration with glycyl dipeptide. The negative sign indicates the co-solutes act a structure breaker.

1. Introduction

The molecular foundation of life rests on the operation of biological macro-molecules, mostly nucleic acids and proteins. Peptides and proteins are also economically significant since they are deployed as nutrition factors and flavor enhancers at a large scale. We ingest them up, assimilate them and use their building blocks – namely the essential amino acids that we cannot generate on our own – to form fresh proteins that play different roles in our biological system, such as hormones, enzymes, and specific receptors. Additionally, many pharmaceuticals drugs such as antibiotics, anti-HIV and cancer drugs are also manufactured by using amino acids. An eminent overview about applications and procedure of production of several amino acids has been reported by Kleemann et al. [1]. The modern cognizance of biological macromolecules is unimaginable without being heedful of the solvent environment [2]. Hydration depicts a vital role in the assemblage of a protein's structure and dynamics. The water molecules are part of the molecular recognition process by proteins or other molecules and also essential to the perception of the activity of enzyme proteins [3–5]. Solute–water interactions immensely influence the conformational sampling of peptides [2]. Specifically, protein folding relies on the presence of water and particularly on hydrophobic effect [6–8] and, in peptides, secondary structure preferences are determined by interactions present between solvent and peptides [9].

On the other hand, in more environmentally friendly technologies, ionic liquids (ILs) are emerging as an excellent choice to substitute volatile organic solvents. ILs have been conceded as important innovated solvents accommodating specific properties including high density, high heat capacity, high thermal stability, extremely low volatility, non-flammability, and wide temperature range for liquid state [10–12].

The interaction of water with biomolecules is an intricate issue that has been reviewed for many decades [13–18]. While the investigation of bio molecular solvation in ionic liquids remains the focus of current research efforts [19–22]. A more precise exploration of physical and thermodynamic properties of these novel systems can provide new insights for further new practices of these mixtures. In the present study, our previous work [23] has been extended by modifying the anionic part of ionic liquid from [Cl^-] to [Br^-], to achieve a better understanding of some structure – property correlation of these mixtures. The novelty of the present work lies in the fact that there exists no report involving the behavior of glycine and glycyl dipeptide at different concentrations

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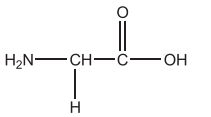
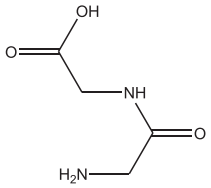
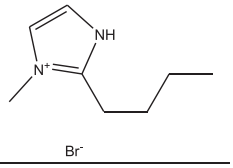
Table 1
Provenance, purity method, purity, CAS number and structure of the chemicals used in the study.

Material	Provenance	Purification method	Mass fraction purity	CAS no.	Structure
Glycine	Merck, Germany	Vacuum drying	>0.99	56-40-06	
Glycyl dipeptide	Merck, Germany	Vacuum drying	>0.99	556-50-3	
1-Butyl-3-methylimidazolium bromide	Sigma Aldrich, USA	Vacuum drying	>0.97	85100-77-2	

of used IL. Moreover, the data of density and speed of sound, and their derived parameters give valuable information regarding the intermolecular interactions between solute and solvent. Along with, such studies can be of great importance not only in the field of solution thermodynamics but in the creation of a new set of data that can help in the development of several chemical and biochemical applications. With this view in mind, we have undertaken the present work. Therefore, in this work, the experimental density and speed of sound of glycine and glycylglycine have been measured in aqueous solution of 1-butyl-3-methylimidazolium bromide, [C_4mim][Br] at temperatures $T =$ (288.15, 298.15 and 308.15) K. The data has been used to compute other parameters like apparent molar volume, apparent molar isentropic compression, partial molar volume, and partial molar isentropic compression at infinite dilution. These thermodynamically derived parameters have been used to figure out transfer parameters, limiting apparent molar expansivity, Hepler's constant and hydration numbers for amino acid and its dipeptide in aqueous [C_4mim][Br].

2. Experimental

2.1. Materials and methods

The provenance, purity method, purity, CAS number and structure of the chemicals used in this study have been mentioned in Table 1. 1-Butyl-3-methylimidazolium bromide, [C_4mim][Br] has been dried overnight at 70 °C under high vacuum. The water content of the ionic liquid was determined using a microprocessor based automatic Karl-Fisher Titrator and it was found to be <350 ppm. The ionic liquid [C_4mim][Br] has also been characterized by ^{1}H NMR (Bruker 300 MHz) and FT-IR (ABB MB3000) to confirm the absence of any major impurities in the current study. Millipore quality freshly degassed water (specific conductance $<10^6$ S·cm^{-1}) has been used to prepare all aqueous solutions. All the solutions were prepared by mass fraction at room temperature in air tight glass vials by using an analytical balance (A&D Co. limited electronic balance (Japan, model GR-202)) having a precision of 0.01 mg. The density (ρ) and speed of sound (u) of the solutions were measured simultaneously by using vibrating –tube digital density and speed of sound analyzer (Anton Paar, DSA 5000 M) at $T =$ (288.15, 298.15 and 308.15) K and at atmospheric pressure. The calibration of instrument was done according to instrument manual by using double distilled deionized, and degassed water, and dry air at atmospheric pressure. The uncertainties of measurements for the molality of binary mixture, density and speed of sound are $\pm 10\cdot10^{-6}$ mol·kg^{-1}, $\pm 5\cdot10^{-3}$ kg·m^{-3} and ± 0.5 m·s^{-1}, respectively.

Table 2
Densities ρ and speeds of sound u for (glycine/glycyl dipeptide + [C_4mim][Br] systems at different temperatures.

m/mol·kg^{-1}	$\rho \cdot 10^{-3}$/kg·m^{-3}			u/m·s^{-1}		
	288.15 K	298.15 K	308.15 K	288.15 K	298.15 K	308.15 K
Glycine + 0.1000 mol kg^{-1} [C_4mim][Br]						
0.0000	1.00335	1.00116	0.99798	1473.4	1502.1	1524.2
0.0503	1.00499	1.00275	0.99954	1476.6	1505.2	1527.0
0.1012	1.00662	1.00434	1.00110	1479.7	1508.2	1529.8
0.2004	1.00978	1.00741	1.00411	1485.6	1513.7	1534.8
0.3000	1.01286	1.01045	1.00709	1491.2	1518.8	1539.3
0.3996	1.01589	1.01343	1.01004	1496.3	1523.7	1543.9
0.4993	1.01888	1.01638	1.01295	1501.3	1528.4	1548.2
0.6003	1.02185	1.01933	1.01583	1506.1	1532.9	1552.3
0.6993	1.02470	1.02216	1.01863	1510.7	1537.1	1555.9
0.7993	1.02754	1.02497	1.02142	1514.9	1541.0	1559.7
Glycine + 0.3000 mol kg^{-1} [C_4mim][Br]						
0.0000	1.01062	1.00822	1.00493	1495.6	1520.6	1537.7
0.0499	1.01219	1.00976	1.00644	1497.6	1522.5	1539.5
0.1005	1.01378	1.01131	1.00797	1499.8	1524.6	1541.5
0.2008	1.01690	1.01437	1.01097	1504.3	1528.9	1545.4
0.2999	1.01995	1.01734	1.01390	1508.8	1533.4	1549.9
0.4000	1.02300	1.02032	1.01683	1513.8	1538.3	1554.5
0.5002	1.02602	1.02327	1.01973	1519.4	1543.7	1559.6
0.5982	1.02893	1.02613	1.02255	1524.5	1549.0	1564.7
0.6994	1.03191	1.02904	1.02543	1530.4	1554.7	1570.2
0.7999	1.03484	1.03191	1.02826	1537.0	1561.4	1576.5
Glycyl dipeptide + 0.1000 mol kg^{-1} [C_4mim][Br]						
0.0000	1.00338	1.00118	0.99800	1470.0	1500.2	1520.8
0.0459	1.00556	1.00333	1.00011	1475.5	1505.1	1525.2
0.1000	1.00811	1.00583	1.00257	1481.3	1510.3	1529.9
0.1497	1.01041	1.00810	1.00480	1485.9	1514.8	1533.9
0.1995	1.01270	1.01035	1.00701	1490.2	1518.8	1537.4
0.2508	1.01504	1.01264	1.00927	1493.6	1522.2	1540.7
0.2998	1.01724	1.01481	1.01140	1496.2	1525.3	1543.7
Glycyl dipeptide + 0.3000 mol kg^{-1} [C_4mim][Br]						
0.0000	1.01395	1.01147	1.00811	1499.8	1524.2	1541.1
0.0459	1.01609	1.01350	1.01011	1503.4	1527.6	1544.5
0.0996	1.01863	1.01589	1.01244	1507.6	1531.6	1548.5
0.1498	1.02102	1.01823	1.01468	1511.7	1535.4	1552.1
0.1996	1.02344	1.02058	1.01693	1515.7	1539.1	1555.7
0.2512	1.02592	1.02305	1.01928	1520.0	1543.1	1559.5
0.3017	1.02841	1.02545	1.02158	1524.2	1547.0	1563.0

m stands for the molalities of glycine and glycyl dipeptide in aqueous solutions of ionic liquid which represents that the solutions of glycine and glycyl dipeptide in (water + ionic liquid) were prepared on the molal basis (i.e.no. of moles of glycine/glycyl dipeptide dissolved in 1000 g of aqueous ionic liquid solution).