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Thermodynamics of the interactions of some amino acids and peptides with dodecyltrimethylammonium bromide and tetradecyltrimethylammonium bromide

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ABSTRACT

The values of apparent molar volume $V_{2,\phi}$ and apparent molar adiabatic compressibility $K_{S,2,\phi}$ of amino acids glycine, L-alanine, DL-α-amino-n-butyric acid, L-valine, L-leucine and peptides glycyl-glycine, glycyl-glycyl-glycine and glycyl-leucine have been determined in aqueous solutions of cationic surfactants dodecyltrimethylammonium bromide (DTAB) and tetradecyltrimethylammonium bromide (TTAB) by means of density and sound velocity measurements. The heat evolved or absorbed (q) during the course of interactions of amino acids and peptides with the aqueous solutions of surfactants were determined by isothermal titration calorimetry at $T = 298.15$ K. The values of standard partial molar volume $V^0_{2,m}$ and standard partial molar adiabatic compressibility $K^0_{s,2,m}$ at infinite dilution were calculated from the values of $V_{2,\phi}$ and $K_{S,2,\phi}$. Similarly the values of limiting enthalpies of dilution ($\Delta_{dil}H^0$) of the amino acids/peptides were calculated from heat evolved or absorbed during calorimetric experiments. The standard partial molar quantities of transfer from water to aqueous surfactant solutions have been used to identify the interactions of amino acids and peptides with surfactants in terms of ionic–ionic, ionic–hydrophobic and hydrophobic–hydrophobic group interactions.

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1. Introduction

Protein–surfactant interactions have been a focus of studies for a long time [1–4]. It is known that protein–surfactant interactions play very important role in industrial, biological, pharmaceutical, and cosmetic applications [5,6]. Surfactants are used for protein molecular weight determination [7], membrane protein solubilization [8], and crystallization [9]. Binding of surfactants to proteins alters intermolecular forces which maintain the secondary and tertiary structure, thereby producing conformational changes [10,11]. Surfactants can interact directly or indirectly with the proteins through different physicochemical mechanisms such as electrostatic or hydrophobic interactions [12–14]. Surfactants may either bind to protein or initiate its unfolding or only bind and retain its tertiary structure intact [15]. The conformational stabilization of the protein in surfactants is related to the nature of solute-solute and solute-solvent interactions. Therefore a detailed understanding of the interactions of the intact proteins and the constituents of proteins with surfactants is essential. Studies on the interactions of model compounds such as amino acids and peptides with surfactants can help in understanding the fine details of protein–surfactant interactions [16–20].

In this work, we have investigated the effect of the cationic surfactants tetradecyltrimethylammonium bromide (TTAB, cmc-$3.7 \cdot 10^{-3}$ mol dm^{-3}) [21] and dodecyltrimethylammonium bromide (DTAB, cmc-$15 \cdot 10^{-3}$ mol dm^{-3}) [22] on some amino acids and peptides using densimetry, sound velocity and calorimetric measurements. Volumetric measurements can be used to investigate the hydration properties of charged (oppositely charged amino and carboxyl termini), polar (a peptide group), and non-polar (a methylene group) groups of α-amino acids [23]. Post micellar concentrations of surfactants TTAB and DTAB have been selected and various physico-chemical parameters, such as partial molar volume, partial molar adiabatic compressibility, and enthalpy of dilution have been evaluated. The corresponding transfer properties have been discussed in terms of various types of intermolecular interactions, to understand the origin and nature of amino acids/peptides–surfactant interactions both qualitatively and quantitatively.

2. Experimental

2.1. Materials

The amino acids glycine, L-alanine, DL-α-amino-n-butyric acid (α-ABA), L-valine, L-leucine and peptides glycyl-glycine,

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glycyl-glycyl-glycine, glycyl-leucine were procured from Sigma Aldrich Co., USA. The surfactants tetradecyltrimethylammonium bromide (TTAB) and dodecyltrimethylammonium bromide (DTAB) were procured from Tokyo Chemical Industry Co., Japan. All the amino acids and peptides were dried over P_2O_5 for at least 72 h and used without further purification. Moisture contents were determined by Karl Fischer analysis and the dry weights of these samples were corrected wherever required. The relative molar mass, moisture content, and purity of these compounds as listed by the vendors are given in table 1. All the solutions were prepared in water that was double distilled, deionized using a Cole-Parmer Barnstead mixed-bed ion exchange resin column and then degassed. All of the mass determinations were done on a Sartorius BP 211D digital balance which had readability of 0.01 mg.

2.2. Methods

Density and sound velocity measurements

The densities and sound velocities of solutions were measured using digital density and sound velocity analyser DSA 5000 purchased from Anton Paar GmbH, Austria. The instrument determines two independent physical properties with the same sample as it is equipped with a density cell and sound velocity cell thus combining the oscillating U-tube method with highly accurate measurement of sound velocity. The temperature of the measurements was stable to within 0.01 K. The chemical calibration of the densimeter was performed by measuring the values of apparent molar volume and apparent molar adiabatic compressibility of aqueous sodium chloride solutions at different values of molality and comparing with the literature values [24], which had excellent agreement. The maximum uncertainties in the density and sound velocity measurements were observed to be $3 \cdot 10^{-6}$ g · cm^{-3} and 0.03 m · s^{-1}, respectively.

Isothermal titration calorimetry

Isothermal titration calorimetric measurements were performed at T = 298.15 K on Nano ITC (TA Instruments, New Castle, DE, USA). All the solutions were thoroughly degassed prior to the experiments. Titrations were carried out using 250 μL syringe filled with aqueous amino acids or peptides solutions with a stirring speed of 250 rpm in all the experiments. The sample cell of 950 μL capacity was filled with 0.1 mol · kg^{-1} aqueous surfactant solutions and the reference cell was filled with water. Titrations of aqueous amino acids and peptides were performed using 0.2 mol · kg^{-1} of glycine, alanine, α-amino-n-butyric acid, 0.05 mol · kg^{-1} valine, leucine, glycyl-leucine, and 0.025 mol · kg^{-1} glycyl-glycine and glycyl-glycyl-glycine. Titrations consisted of 25 consecutive injections of aqueous amino acids or peptides with 20 s duration each and 240 s interval between every successive injection. The ITC experiments provided a set of values of the heat liberated or absorbed at different molalities of amino acids or peptides in the solutions. The limiting heat of dilution ($\Delta_{dil}H^0$) of the aqueous amino acid and peptide solution was calculated by fitting the values of the measured heat (q) to the following equation,

$$q = \Delta_{dil}H^0 + mS_V. \tag{1}$$

Here m is the molality of the solution and S_V is the empirical slope. The data which showed linear molality dependence were fitted to the above equation. In other cases, the data points were fitted to an appropriate polynomial equation to obtain the values of $\Delta_{dil}H^0$.

3. Results and discussion

The value of apparent molar volume ($V_{2,\phi}$) of amino acids and peptides in aqueous surfactant solutions was determined from the measured density ρ using equation (2). The value of isentropic compressibility of the aqueous solution (κ_S) was calculated from the speed of sound, u, using the Newtonian–Laplace equation (3). The value of apparent molar adiabatic compressibility, $K_{S,2,\phi}$ was determined by using equation (4).

$$V_{2,\phi} = \frac{M}{\rho} - \frac{(\rho - \rho_o) \times 10^3}{m\rho\rho_o}, \tag{2}$$

$$\kappa_S = \frac{1}{u^2\rho}, \tag{3}$$

$$K_{S,2,\phi} = \frac{\kappa_S M}{\rho} + \frac{1000(\kappa_s^0\rho - \kappa_S\rho_0)}{m\rho\rho_0} \tag{4}$$

Here M is the molar mass of the solute in g · mol^{-1}, m is the molality of the solution in mol · kg^{-1}, ρ_o is the density of water or the reference solvent in units of g · cm^{-3}. The κ_S^0 is the isentropic compressibility of water or the reference solvent at T = 298.15 K. In so far as the isentropic compressibility is dependent on the ultrasonic speed, the latter may be considered as a thermodynamic property in the sole case when a negligible amount of ultrasonic absorption of the acoustic waves of low frequency and of low amplitude is observed.

The values of measured density (ρ), apparent molar volume ($V_{2,\phi}$), speed of sound (u), isentropic compressibility (κ_S), and apparent molar adiabatic compressibility ($Ks_{,2,\phi}$) of amino acids and peptides at different molalities at T = 298.15 K, in 0.1 mol · dm^{-3} aqueous DTAB and TTAB surfactant solutions are given in tables S1 and S2, respectively. The values of the measured thermodynamic quantities have been plotted as a function of molality in figures 1–4. In the case where the values of $V_{2,\phi}$ were found to be molality dependent, the values of standard partial

TABLE 1
Compounds used in this study with their Molecular formula, Molar mass (M), Source (S = Sigma Aldrich Co, USA, SRL = Sisco Research Laboratories, India, F = Fluka Analytical, Japan, TCI= Tokyo Chemical Industry Co, Japan), CAS number, mass fraction moisture content (w) and their mole fraction purity (x) as reported by the vendors.

Compound	Molecular formula	M	Source	CAS No.	w	mass fraction purity
Glycine	$C_2H_5NO_2$	75.07	S	56-40-6	0.0004	⩾0.99
L-alanine	$C_3H_7NO_2$	89.09	S	302-72-7	0.0006	⩾0.99
DL-α-amino-n-butyric acid	$C_4H_9NO_2$	103.12	SRL	2835-81-6	0.0004	=0.99
L-valine	$C_5H_{11}NO_2$	117.15	S	72-18-4	0.0006	⩾0.98
L-leucine	$C_6H_{13}NO_2$	131.12	S	61-90-5	0.0007	⩾0.98
Glycyl-glycine	$C_4H_8N_2O_3$	132.12	F	556-50-3	0.0009	⩾0.99
glycyl-glycyl-glycine	$C_6H_{11}N_3O_4$	189.17	S	556-33-2	0.0010	⩾0.99
glycyl-leucine	$C_8H_{16}N_2O_3$	188.23	S	869-19-2	0.0008	>0.99
DTAB	$C_{15}H_{34}BrN$	308.35	TCI	1119-94-4	0.0010	>0.98
TTAB	$C_{17}H_{38}BrN$	336.40	TCI	1119-97-7	0.0015	>0.98

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