

The limiting partial molar volume and transfer partial molar volume of glycylglycine in aqueous sodium halide solutions at 298.15 K and 308.15 K

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Abstract

Apparent volumes V_{ϕ} of glycylglycine in aqueous NaX ($X = F^{-}$, Cl^{-} , and Br^{-}) solutions have been obtained from densities of their solutions at 298.15 K and 308.15 K measured by using a precise vibrating-tube digital densimeter. These values have been utilized in conjunction with the values in water to deduce partial molar volumes of transfer $\Delta_{\text{trs}}V_{\phi}^{\circ}$ from water to different aqueous NaX solutions. $\Delta_{\text{trs}}V_{\phi}^{\circ}$ values are positive. The interpretation is that these results arise from the dominant interaction of the NaX with the charged centers of glycylglycine. The results show that $\Delta_{\text{trs}}V_{\phi}^{\circ}$ depend less on the temperature. Hydration numbers and interaction coefficients have been calculated from V_{ϕ}° and $\Delta_{\text{trs}}V_{\phi}^{\circ}$ values and the values have been interpreted in terms of various interactions. © 2005 Elsevier Ltd. All rights reserved.

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1. Introduction

The partial molar volume of proteins is a characteristic parameter that has been used to elucidate several processes such as the protein conformation changes, protein aggregation or polymerization [1–6]. Because of the structure complexities of proteins, it is extremely difficult to investigate thermodynamic properties directly. It has been common practice to use amino acids and oligopeptides as model compounds since they make up of the protein structures [7–10].

Most of the previous studies on oligopeptides have been restricted to water [11–14]. However, biological fluids are not pure water. Investigating the influence of solvents is therefore important. The properties of proteins such as their structure, solubility, denaturation, activity of enzymes, etc. are greatly influenced by electrolytes [15–18].

Though there are some papers investigating this property of glycylglycine in aqueous NaCl solutions [19,20], no systematic studies exists on the voluminal properties of oligopeptides in electrolyte solutions. For complete understanding of the influence of electrolytes on oligopeptides, in this paper, we present the densities ρ , apparent volumes V_{ϕ} and infinite dilution apparent molar volume V_{ϕ}° in aqueous NaX solutions at $T = 298.15$ K and 308.15 K. Only sodium salts have been chosen for this part of the isolated study to observe the relative effects of the change of anion of the electrolyte.

2. Experimental

2.1. Materials

Glycylglycine (mass fraction ≥ 0.98) was procured from China Medicine (Group) Shanghai Chemical Reagent Corporation. It was dried in a DZF-6020 model

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dry box of vacuum for six hours at 60 °C and stored over silica gel in a vacuum desiccator for 48 h before use. Sodium Chloride (mass fraction ≥ 0.995) procured from Ningbo Chemical Reagent Factory, sodium fluoride (mass fraction ≥ 0.98) procured from Dongyang Chemical Factory, and sodium bromide (mass fraction ≥ 0.985) procured from Shanghai Reagent Factory were purified by two recrystallizations from distilled and deionized water obtained by a quartz sub-boiling purifier, and were dried at 110 °C. They were also stored over silica gel in a vacuum desiccator for 48 h before use.

Solutions of different compositions were prepared by weight using a Mettler AE 200 analytical balance with a precision of ± 0.0001 g. All liquids were degassed ultrasonically.

2.2. Density measurements

The densities of solutions were determined by a vibrating-tube digital densimeter (DMA55 Anton Paar) thermostated to better than ± 0.01 K (HAAKE C). The precision of the densimeter was ± 0.00001 $\text{g} \cdot \text{cm}^{-3}$. The densimeter was calibrated with twice distilled water and dried air. The density of water at 298.15 K and 308.15 K were, respectively, taken as 0.99705 $\text{g} \cdot \text{cm}^{-3}$ and 0.99403 $\text{g} \cdot \text{cm}^{-3}$ [21]. The density of air was 1.1845 $\cdot 10^{-3}$ $\text{g} \cdot \text{cm}^{-3}$ and 1.1460 $\cdot 10^{-3}$ $\text{g} \cdot \text{cm}^{-3}$ [22].

The average of triplicate measurements was as the final result.

3. Results

3.1. The partial molar volume at infinite dilution and transfer partial molar volume

Apparent molar volumes, V_ϕ , were calculated from the density values using the equation:

$$V_\phi = M/\rho - (\rho - \rho_0)/(m\rho\rho_0), \quad (1)$$

where M is the molar mass of the solute (glycylglycine), m is the molality of the solute in aqueous NaX solution; ρ is the density of solution (glycylglycine, NaX, and water), and ρ_0 is the density of aqueous NaX solution.

Estimated uncertainties in apparent molar volumes, δV_ϕ , were calculated using the equation reported by Hedwig [23]

$$\delta V_\phi = -(M + 1/m)\delta\rho/\rho^2. \quad (2)$$

The uncertainty in solution density, $\delta\rho$, was estimated to be $2 \cdot 10^{-5}$ $\text{g} \cdot \text{cm}^{-3}$. In using the equation (2), the contributions to δV_ϕ arising from uncertainties in solution molalities are assumed to be negligible which are much smaller (0.03% to 0.15%) than that arising from the uncertainties in density.

The densities and apparent molar volumes of the glycylglycine and the uncertainties are presented in table 1.

Partial molar volumes at infinite dilutions were obtained by least squares fitting to the equation:

$$V_\phi = V_\phi^\circ + S_v m, \quad (3)$$

where, S_v is the experimental slope, and m is the molality of the solute (glycylglycine) in mixtures. Apparent molar volumes of glycylglycine were found to be a perfect linear function of molality over the molality range studied. In some papers [20,24,25], apparent molar volumes were found to be independent of solution molality, and partial molar volumes at infinite dilutions were calculated by averaging apparent molar volumes over the investigated molality range.

The transfer parameters were calculated as defined by

$$\Delta_{\text{trs}} V_\phi^\circ \{\text{water to NaX(aq)}\} = V_\phi^\circ \{\text{in NaX(aq)}\} - V_\phi^\circ \{\text{in water}\}. \quad (4)$$

The partial molar volumes at infinite dilutions along with the stand deviations of fitting to the equation (3) and the transfer partial molar volumes values are presented in table 2.

3.2. The hydration number

The partial molar volume at infinite dilution of a nonelectrolyte can be divided into two parts as follows [26]

$$V_\phi^\circ = V_{\text{int}} + V_{\text{elect}}, \quad (5)$$

where V_{int} is the intrinsic molar volume of the nonelectrolyte solute, and V_{elect} is the electrostriction partial molar volume due to the hydration of the nonelectrolyte.

Shahidi *et al.* [27] reported the intrinsic molar volume could be estimated by using the molar volume of nonelectrolyte crystal

$$V_{\text{int}} = (0.7/0.634)V_{\text{crist}}, \quad (6)$$

0.7 is the fill density of crystal molecule, 0.634 is the fill density of the accumulation balls, which are ruleless, and V_{crist} is the molar volume of the nonelectrolyte crystal calculated by the equation:

$$V_{\text{crist}} = M/\rho_{\text{crist}}, \quad (7)$$

where ρ_{crist} is the crystal density of glycylglycine which is 1.534 $\text{g} \cdot \text{cm}^{-3}$ [28] at $T = 298.15$ K. Since crystal density has a very small change with temperature, we assume the ρ_{crist} value at 308.15 K is approximately equal to the value at 298.15 K.

Millero *et al.* [29] reported that the relationship of the electrostriction volume and the hydration number of nonelectrolyte in solution could be expressed as

$$V_{\text{elect}} = N_h(V_c^\circ - V_b^\circ), \quad (8)$$

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