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Effect of temperature on the partial molar volume, isentropic compressibility and viscosity of DL-2-aminobutyric acid in water and in aqueous sodium chloride solutions

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Density, sound velocity and viscosity of DL-2-aminobutyric acid in water and in aqueous sodium chloride solutions have been measured at temperatures of (293.15, 298.15, 303.15, 308.15 and 313.15) K. The experimental results were used to determine the apparent molar volume and the apparent molar compressibility as a function of composition at these temperatures. The limiting values of both the partial molar volume and the partial molar adiabatic compressibility at infinite dilution of DL-2-aminobutyric acid in water and in aqueous sodium chloride solutions were determined at each temperature. The experimental viscosity values were adjusted by a least-squares method to a second order equation as proposed by Tsangaris-Martin to obtain the viscosity *B* coefficient which depends on the size, shape and charge of the solute molecule.

The influence of the temperature on the behaviour of the selected properties is discussed in terms of both the solute hydration and the balance between hydrophobic and hydrophilic interactions between the acids and water, and the effect of the sodium chloride concentration.

1. Introduction

Physicochemical properties of aqueous solutions of small organic compounds such as amino acids in water and in aqueous solutions of salts are of considerable interest in the study of hydrophobic and hydrophilic interactions between these solutes and water and their effect on water structure [1,2]. Amino acids have been considered model compounds that can give useful information to understand the behaviour of proteins and the role of solvent structure in the denaturation process. In particular, volumetric, molar compressibility and viscometric properties of aqueous solutions of amino acids are important for the information they give on the nature of interactions between non-polar and polar groups with water and their effect on water structure [3,4]. This information is also fundamental to understand whether and to what extent a given type of interaction determines the native conformation of a protein [5–12].

In the case of amino acids the information available in the literature is limited and even though the effect of temperature has been used to obtain information about solute hydration, most studies have been done with small naturally occurring amino acids however, few data are reported in literature for linear hydrocarbon chain amino acids such as DL-2-aminobutyric acid, especially at temperatures different from 298.15 K.

As a continuation of an earlier work on the thermodynamic properties of amino acids in aqueous solution, in the actual study we present the apparent molar volume, the apparent molar compressibility and the viscosity of DL-2-aminobutyric acid (α-amino butyric acid) in water and in aqueous sodium chloride solutions as a function of the concentration at temperatures of (293.15, 298.15, 303.15, 308.15 and 313.15) K [4,13–19]. The DL-2-aminobutyric acid (Fig. 1) was selected because it has a linear hydrocarbon chain and previous works have shown that in aqueous solutions the behaviour of this amino acid is dominated by hydrophobic hydration, while the smaller amino acids, glycine and alanine, the hydrophilic hydration is the dominant interaction [4,15,16,19].

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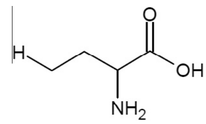

Fig. 1. Chemical structure of the α-aminobutyric acid.

It is well known that the presence of electrolytes affects the behaviour of amino acids in solution and consequently, in biological and industrial process in which they are involved. In this work, sodium chloride was chosen as electrolyte because aqueous saline solutions are present as the environment of most molecules with biological interest.

The influence of the temperature on the behaviour of volumetric properties of aqueous solutions of DL-2-aminobutyric acid in water and in aqueous sodium chloride solutions has been used to obtain information about the effect of the salt on solute hydration.

2. Experimental

2.1. Materials

The characteristics of the reagents used are presented in Table 1. The mass fraction purity is reported according to the certificates of analysis. DL-2-aminobutyric acid and sodium chloride were used without further purification. They were dried under vacuum at room temperature and kept in a desiccator at least 48 h before use. Water was purified using a Barnstead Easy-Rodi DI 3321 system and degassed before use; the resulting water showed a conductivity less than 1.5 $\mu S \cdot m^{-1}$ [20,21]

All solutions were prepared by weighing both the solute and water in a Mettler balance AT-261 dual range with readability of 1×10^{-5} g and reproducibility better than 1×10^{-5} g in the lower range.

2.2. Methods

2.2.1. Density and sound velocity measurements

Density and sound velocity of the aqueous solutions were measured using a vibrating U-tube densimeter, Anton Paar DSA 5000, with a temperature control better than ±0.001 K and a working frequency of 3 MHz. The densimeter was calibrated with dry air and purified water at 293.15 K. Values of the density and sound velocity reported are the average of three independent measurements with an uncertainty of 0.150 $(kg \cdot m^{-3})$ for density and 2 $(m \cdot s^{-1})$ for sound velocity.

Values of the apparent molar volume ϕ_V were calculated from the density results using Eq. (1):

$$\varphi_V = \frac{M}{\rho} + \frac{(\rho_0 - \rho)10^3}{m\rho\rho_0} \tag{1}$$

where M is the molar mass of the solute (DL-2-aminobutyric acid), m its molal concentration in the aqueous solution, ρ_o is the density of the solvent (either pure water or aqueous solution of sodium chloride) and ρ is the solution density.

The apparent molar adiabatic compressibility, ϕ_K, of the amino acid in water and in the NaCl aqueous solutions were determined, respectively, from the density ρ, and adiabatic compressibility, β_S, of the corresponding solution by using the equation

$$\varphi_K = \frac{M\beta_s}{\rho} + \frac{(\beta_s\rho_0 - \beta_s^0\rho)10^3}{m\rho\rho_0} \tag{2}$$

where β_S^o is the adiabatic compressibility of the solvent. The adiabatic compressibility β_S of the aqueous solution at each temperature was calculated from both the sound speed, u, and density measurements by means of the Newton-Laplace equation [22]

$$\beta_S = 1/\rho u^2 \tag{3}$$

2.2.2. Viscosity measurements

Viscosity was determined using two modified suspended-level Ubbelohde capillary viscometers calibrated with water at the selected temperatures. Efflux times were measured using an infrared sensor that operated an electronic chronometer in an optical fibre arrangement. For each solution, the efflux time represents the average of at least five independent measurements. Reproducibility of efflux times was, in all cases, better than 0.05%. All measurements were carried out in a constant temperature bath with temperature controlled to ±0.01 K.

The viscosity values were obtained from the relation:

$$\eta = \alpha\rho t - \beta\rho/t \tag{4}$$

where α and β are the viscometer constants, ρ is the density and t the efflux time. The relative viscosity, $\eta_r = \eta/\eta_o$, was calculated from the solution and the solvent viscosities, η and η_o, respectively. The viscometer constants were determined by calibration using water at different temperatures and their values are $\alpha = 3.29 \times 10^{-3}$ $cm^2 \cdot s^{-2}$ and $\beta = 9.176$ cm^{-2}. The relative standard uncertainty of the viscosity measurement is 1.0%.

The values of density, viscosity and the adiabatic compressibility of water, at each temperature, used in calibration were taken from the literature [20,23,24].

3. Results and discussion

The data for density ρ, sound velocity u, apparent molar volume φ_V, apparent molar compressibility φ_K and viscosity η at temperatures of (293.15, 298.15, 303.15, 308.15 and 313.15) K are presented in the supporting material of this paper for the thermodynamic properties of α-aminobutyric acid in water. A graphical comparison between our results and some literature values is included [25–27] in Figs. S4–S6 in the Supporting Material. The values which we obtained for the properties of the aqueous solutions of NaCl used as solvent, are in good agreement with previously published values [24,28,29]. The differences observed are in most cases within the experimental uncertainty, as can be observed in the graphical comparison in Figs. S1–S3 included as Supporting Material.

3.1. Apparent molar volume

The apparent molar volume of DL-2-aminobutyric acid in water and in the aqueous solutions of sodium chloride shows weak concentration dependence at all the selected temperatures. It can be observed that its value increases as the concentration of sodium

Table 1
Sample provenance and mass fraction purity.

Chemical name	Source	Mass fraction purity	Purification method	Final mass fraction purity	Analysis method
DL-2-Aminobutyric acid	Sigma	$w > 0.99$	None	–	–
Sodium chloride	Merck	$w = 0.995$	None	–	–