



# Volumetric and viscometric study of amino acids in aqueous sorbitol solution at different temperatures



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## ABSTRACT

Densities ( $\rho$ ) and viscosities ( $\eta$ ) of glycine, L-alanine, L-valine, L-threonine and L-arginine in (0.2, 0.4, 0.6, 0.8 and 1.0) mol · kg<sup>-1</sup> aqueous sorbitol solutions have been measured at  $T = (293.15, 303.15, 313.15$  and  $323.15)$  K under atmospheric pressure. The apparent molar volume ( $V_{\phi}$ ) and the limiting partial molar volumes of amino acids ( $V_{\phi}^0$ ) were calculated through the density data. And the limiting partial molar volumes of transfer ( $\Delta_{tr}V_{\phi}^0$ ) and interaction coefficients  $V_{ab}$ , and  $V_{abb}$  were also determined. The extended Jones–Dole equation was used to correlate the viscosities in order to obtain viscosity *B*-coefficient and the free energies of activation per mole of solvent ( $\Delta\mu_1^{0\ddagger}$ ) and solute ( $\Delta\mu_2^{0\ddagger}$ ). The limiting partial molar volume of transfer and the free energies of activation per mole of both solvent ( $\Delta\mu_1^{0\ddagger}$ ) and solute ( $\Delta\mu_2^{0\ddagger}$ ) were discussed on the basis of the co-sphere overlap model and transition state theory, respectively. The hydration number of amino acids was computed using the obtained limiting partial molar volume and viscosity *B*-coefficient. Additionally, the group contribution method was applied to determine the respective contribution of (NH<sub>3</sub><sup>+</sup>, COO<sup>-</sup>), CH<sub>2</sub>, OH and CNHNNH<sub>2</sub> to  $V_{\phi}^0$  and *B*-coefficient.

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## 1. Introduction

It is well known that polyhydroxy compounds play a very significant role in stabilizing the native state of a globular protein [1,2]. The non-covalent interactions between polyhydroxy compounds and protein, such as electrostatic and hydrophobic interactions, are the crucial factors that determine the complex conformational and configurational structures of protein and remarkably affect their denaturalisation, solubility, as well as folding/unfolding behaviour [3,4]. Due to huge and complicated molecule structure of the protein, the study on the molecular interactions remains still challenging.

To get insight into the mechanism of the molecular interactions, amino acids, as the basic building blocks of protein and the most important protein model compound, are quite appropriate to explore the molecular interactions. Recently, a number of investigations on the interactions of amino acids and polyhydroxy compounds have been reported [5–13].

As a typical polyhydroxy compound, sugar alcohol is usually used as sugar replacer due to its low calorie and little effect on blood sugar level [14], and thus has been used widely in the phar-

maceutical and food industries. Sorbitol((2S,3R,4R,5R)-hexane-1,2,3,4,5,6-hexol) derived from glucose by the enzyme aldose reductase [15], is an organic solute in the cells of human body. Moreover, sorbitol is generally known to enable to provide the stability for lots of proteins [4]. However, to our best knowledge, few studies on thermodynamic properties of (amino acids + sugar alcohol + water) solutions were implemented. Liu *et al.* [16] studied the enthalpy of dilution and the volumetric properties of *N*-glycylglycine in aqueous xylitol solutions at  $T = 298.15$  K. Qiu *et al.* [17] presented the transfer enthalpies of amino acids and glycine peptides from water to the aqueous solutions of sugar alcohol at  $T = 298.15$  K. Jha and Kishore [18] reported only the volumetric properties of some amino acids in aqueous sorbitol solutions at  $T = 298.15$  K. For complementing and providing some new material property data, in the paper, the densities and viscosities of glycine, L-alanine, L-valine, L-threonine and L-arginine in aqueous sorbitol solutions of (0.2, 0.4, 0.6, 0.8, 1.0) mol · kg<sup>-1</sup> at  $T = (293.15, 303.15, 313.15, 323.15)$  K were measured. And the apparent molar volume ( $V_{\phi}$ ), transfer partial molar volume ( $\Delta_{tr}V_{\phi}^0$ ), interaction coefficients, viscosity *B*-coefficient, the free energies of activation per mole of solvent ( $\Delta\mu_1^{0\ddagger}$ ) and solute ( $\Delta\mu_2^{0\ddagger}$ ) and the hydration number were further calculated from the measured densities and viscosities. Additionally, the contributions of zwitterionic end groups (NH<sub>3</sub><sup>+</sup>, COO<sup>-</sup>), CH<sub>2</sub> group, OH group and CNHNNH<sub>2</sub> group

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to  $V_{\phi}^0$  and viscosity  $B$ -coefficients were also evaluated. The interactions of (solute + solute) and (solute + solvent) and the structure making/breaking tendency were analysed based on the co-sphere overlap model and transition state theory.

## 2. Experimental

### 2.1. Materials

The analytical-grade reagent sorbitol, glycine, L-alanine, L-valine, L-threonine and L-arginine were obtained from Aladdin Chemical Reagent Co., Ltd. All these materials were used without further purification. The specific details are given in table 1. An electronic balance (FA2204B, Shanghai Jingke, China) with an accuracy of 0.0001 g was used to prepare the binary and ternary solutions. Aqueous sorbitol solutions of (0.2, 0.4, 0.6, 0.8, 1.0) mol · kg<sup>-1</sup> concentrations were prepared using distilled water and then were used as solvent to prepare the ternary mixtures in the molality range of (0 to 0.7) mol · kg<sup>-1</sup> except L-valine from (0 to 0.4) mol · kg<sup>-1</sup> owing to its solubility. The relative uncertainty of the molality is 2% for L-arginine and sorbitol, and is 1% for other amino acids.

### 2.2. Density and viscosity measurements

Densities measurements were carried out at atmosphere pressure using a vibrating tube densimeter (Anton Paar DMA 4500M, Austria), and the temperature was automatically maintained within ±0.03 K during the measurement through two integrated Pt100 platinum thermometers with built-in peltier elements. The uncertainty in density value is ±1 · 10<sup>-4</sup> g · cm<sup>-3</sup>. Triplicate measurements of each sample were conducted to obtain the average value of density. The apparatus was calibrated by the deionized water and dry air, and after each measurement the distilled-water and anhydrous ethanol were used to clean the vibrating tube automatically.

The viscosity of amino acids in aqueous sorbitol solution was measured by means of an iVisc capillary viscometer (LAUDA, Germany), and the Ubbelohde capillary (1834A) with 0.53 mm diameter was supplied by Shanghai Glass Instruments Factory of China. The thoroughly cleaned and dried Ubbelohde capillary was vertically placed in a Lauda Eco Sliver thermostat with uncertainty ±0.05 K. The flow time for each sample was measured by the infrared automatically with an uncertainty of ±0.01 s, and an average of at least four sets of flow time with a deviation of 0.2 s was taken at the specified temperature. Due to all flow time was greater than 100 s, the kinetic energy and the end corrections were found to be negligible.

The viscosity of amino acids in aqueous sorbitol solution was determined using the following equation [19]:

$$\eta/\eta_w = \rho t/\rho_w t_w, \quad (1)$$

where  $\eta$ ,  $\rho$ ,  $t$  and  $\eta_w$ ,  $\rho_w$ ,  $t_w$  are viscosity, density, and flow time of the solution and water, respectively. The densities and viscosities of water were obtained from the reference [20]. The values of viscosity of the binary and ternary solutions are included in table 2, and the relative uncertainty in viscosity is 2%.

## 3. Results and discussion

### 3.1. Volumetric properties

#### 3.1.1. Apparent molar volumes

The densities of amino acids in  $m_b = (0.2, 0.4, 0.6, 0.8, 1.0)$  mol · kg<sup>-1</sup> sorbitol aqueous solutions at  $T = (293.15, 303.15, 313.15, 323.15)$  K are given in table 2. The comparisons of the densities and viscosities for binary solutions (sorbitol + water) with literature values [21,22] are shown in figure 1. The experimental densities and viscosities values show good agreement with the data in literature. Jha reported the densities of (amino acids + sorbitol + water) ternary solutions, but all concentrations of sorbitol in Jha's study (1.1 and 2.6) mol · kg<sup>-1</sup> are higher than that in this paper (0.2 to 1.0) mol · kg<sup>-1</sup>, and the measured temperature (only 298.15 K) in Jha's study is also different from our present work (293.15, 303.15, 313.15 and 323.15) K, thus densities of ternary solutions are only compared qualitatively in Supplementary figures S1 to S3 (Supplementary Information). In Supplementary figures S1 to S3(a), due to the large molality of sorbitol, the literature values for 1.1 mol · kg<sup>-1</sup> sorbitol solutions at  $T = 298.15$  K are larger than our experimental densities for 1.0 mol · kg<sup>-1</sup> sorbitol solutions at  $T = 293.15$  K. In Supplementary figures S1 to S3(b), the Jha's density values for 1.1 mol · kg<sup>-1</sup> sorbitol solutions at  $T = 298.15$  K fall in the middle of two our experimental extrapolated lines for  $T = (293.15$  and  $303.15)$  K respectively, but the values for 2.6 mol · kg<sup>-1</sup> are smaller than the extrapolated values of our experiment. The discrepancies could be due to the difference of the solution preparation method and chemical materials purity, and the extrapolation deviation. Moreover, in the reference [23], the densities of sorbitol in (0.05, 0.15, 0.25, 0.35, 0.50) mol · kg<sup>-1</sup> glycine aqueous solution have been measured at  $T = (288.15, 298.15, 308.15$  and  $318.15)$  K under atmospheric pressure. In our study, the densities of sorbitol in glycine aqueous solutions of (0.1 to 0.7) mol · kg<sup>-1</sup> were measured at  $T = (293.15, 303.15, 313.15, 323.15)$  K. In addition, the molality of sorbitol in the reference is in the range from (0.04979 to 0.21848) mol · kg<sup>-1</sup>, which are mostly smaller than the molality (0.2 to 1.0) mol · kg<sup>-1</sup> in our work. Comparing the reference with our work, only the molality 0.50 mol · kg<sup>-1</sup> of glycine is the same as our experimental molality. Therefore, the density of glycine of 0.50 mol · kg<sup>-1</sup> versus the molality of sorbitol at different temperatures is plotted in Supplementary figure S4 (Supplementary Information). From the Supplementary figure S4, the density values in the literature at  $T = 308.15$  K are lie in between two extrapolated lines of experimental densities at  $T = (303.15$  and  $313.15)$  K, and the values at

**TABLE 1**  
Provenance and mass fraction purity of the chemicals used.

Chemical name	Mass fraction purity <sup>a</sup>	Molar mass/g · mol <sup>-1</sup>	Source	CAS No.
Sorbitol	≥0.98	182.18	Aladdin Chemical Reagent Co., Ltd.	50-70-4
Glycine	≥0.995	75.07	Aladdin Chemical Reagent Co., Ltd.	56-40-6
L-alanine	≥0.99	89.09	Aladdin Chemical Reagent Co., Ltd.	56-41-7
L-valine	≥0.99	117.15	Aladdin Chemical Reagent Co., Ltd.	72-18-4
L-threonine	≥0.99	119.13	Aladdin Chemical Reagent Co., Ltd.	72-19-5
L-arginine	≥0.98	174.20	Aladdin Chemical Reagent Co., Ltd.	74-79-3

<sup>a</sup> Declared by the supplier.

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