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Effect of glucose/lactose on the solution thermodynamics of thiamine hydrochloride in aqueous solutions at different temperatures

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ABSTRACT

Apparent molar volume, V_ϕ, apparent molar isentropic compression, $K_{\phi,s}$ and viscosity *B*-coefficients have been evaluated for one of the vitamins, thiamine hydrochloride (thiamine-HCl), in aqueous solutions of two carbohydrates, glucose and lactose, at temperatures (293.15–313.15) K from density, speed of sound and viscosity data. Accordingly, limiting apparent molar volume, V^0_ϕ, was obtained from Redlich-Meyer equation whereas limiting apparent molar isentropic compression, $K^0_{\phi,s}$, was calculated on the basis of Debye-Huckel theory. The transfer parameters ($\Delta_{tr}V^0_\phi$, $\Delta_{tr}K^0_{\phi,s}$ and $\Delta_{tr}B$) at infinite dilution, limiting apparent molar expansivity, E^0_ϕ, Hepler's constant, $(\partial^2 V^0_\phi/\partial T^2)_P$, thermal expansion coefficient, α, pair and triplet interaction coefficients and solvation number, S_n, have also been estimated. The viscosity *B*-coefficients and activation parameters have been obtained from Jones-Dole equation and transition state theory. The results have been discussed in terms of competing patterns of interactions prevailing in the solute and solvent.

1. Introduction

Biofluid contains small molecules like sugars, amino acids, vitamins, nucleotides, nucleosides and proteins along with inorganic salts of many metal ions. In order to catalyze oxidation-reduction reaction and various types of group transfer processes, a cofactor is needed by enzymes which may be a metal ion or organic molecule (coenzyme). Vitamins, the absolutely necessary micronutrients of animal diet, are precursors for various coenzymes [1]. They may act or get converted into coenzyme to maintain the health of immune system. Vitamins maintain mental health, immunity and assist in preventing certain chronic diseases. Since ancient times, many diseases due to vitamin deficiencies such as night blindness, scurvy, pellagra, beriberi and rickets have been reported. Vitamins are classified by their biological and chemical activity, as well as by the materials in which they will dissolve.

Thiamine, also known as thiamin or vitamin B_1, is a vitamin found in food and used as a dietary supplement. The water soluble thiamine exists in the form of salt as thiamine hydrochloride ($B_1 \cdot HCl$). In food industry, it is used as a nutritional additive, nutritional source and flavour enhancer [2]. Being a coenzyme or their precursor for several major enzyme complexes, it is an essential constituent for carbohydrate metabolism and genetic regulatory processes [3–4]. It is also requisite for normal function and development of nerves and brain [5]. Since vitamins are not synthesized within the body, these must be supplemented in the food products as a food additive [6]. It has been well documented that non-covalent interactions like ion-dipolar, hydrophilic-hydrophilic, hydrophobic-hydrophobic and hydrophilic-hydrophobic, etc. play an active part for the stabilization of bioactive molecules in solution phase. These interactions are largely affected by the surrounding solvent and cosolute molecules. As a consequence of it, the thermophysical behavior of vitamins is strongly influenced in presence of aqueous cosolutes [7].

Diet consumption can dramatically influence thiamine requirements. The need for thiamine increases as consumption of carbohydrate increases. As mentioned above, since thiamine functions as a coenzyme in the metabolism of carbohydrates, therefore, studies of volumetric, acoustic and transport properties of vitamins in water and aqueous solutions of carbohydrates can provide useful information about their mechanistic action.

The literature survey reveals work on the thermodynamics of amino acids in thiamine-HCl [8], some vitamins in water [9–11] and in various salts [7,12,13]. However, to the best of our knowledge, the thermodynamic study of thiamine-HCl in aqueous solutions of carbohydrates (glucose and lactose) is not available. Hence, in this paper we are reporting the various types of interactions interplaying in thiamine-HCl and aqueous solutions of glucose/lactose based upon apparent and limiting apparent molar volumes, limiting apparent molar

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expansivity, apparent and limiting apparent molar isentropic compression, viscosity B-coefficients, free energy of activation, etc. at T = (293.15 to 313.15) K and 1 atmospheric pressure.

2. Experimental

2.1. Materials

The specification of the chemicals used in this study is given in Table 1. D-(+)-Glucose, thiamine-HCl and α-lactose monohydrate were used as such without further purification. However, these materials were vacuum dried at room temperature followed by storing in desiccator over P_2O_5 before their use, except α-lactose monohydrate. Freshly prepared triply distilled water was used for preparation of aqueous solutions of thiamine-HCl as well as glucose/lactose.

2.2. Methods

The solutions were prepared on molality basis using Mettler Toledo balance (Model: ML204) with an accuracy of ± 0.1 mg. The concentration of thiamine-HCl (solute) was kept within the range of (0 to 0.10) mol kg^{-1}. The solute was then dissolved in water and also in aqueous glucose/lactose (solvent) whose concentration was varied from (0.1 to 0.3) mol kg^{-1}. In order to avoid the exposure to air and evaporation, the solutions were prepared with utmost care and stored in special airtight bottles.

The density of solutions was measured using an Anton Paar densimeter (Model: DMA 5000M). Prior to start, a density check on air/water adjustment was performed at 293 K with triply distilled water followed by dry air at atmospheric pressure. The temperature of the densimeter was controlled to $\pm 1 \times 10^{-3}$ K by a built-in Peltier device. The sensitivity of the instrument corresponds to a precision in density measurements of 1×10^{-3} kg m^{-3}. The uncertainty in the density estimates was found to be within $\pm 5 \times 10^{-3}$ kg m^{-3}. A single crystal variable path multi frequency ultrasonic interferometer (M-82, Mittal Enterprises, India) having stainless steel sample cell with digital micrometer at fixed frequency of 4 MHz was used for measurement of speed of sound. The uncertainty in speed of sound measurements was found to be within ± 0.5 m s^{-1}. An electronic controlled thermostatic water bath (Model: TIC-4000N, Thermotech, India) was used for maintaining the temperature of the solutions to an accuracy of ± 0.01 K. The viscosity of solutions was measured using an Ubbelohde viscometer which was precalibrated with distilled water at different temperatures. The viscometer containing the test liquid was thermostated for about 30 min in a thermostatic water bath in order to avoid the thermal fluctuations. An average of three to four sets of flow time for each solution was taken. A digital stopwatch with an accuracy of ± 0.01 s was used for recording the time of flow for each solution. The accuracy in viscosity measurements was found to be $\pm 1 \times 10^{-6}$ Pa s.

3. Results and discussion

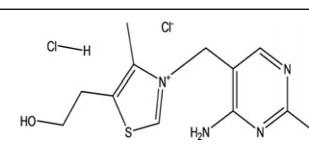
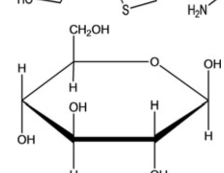
3.1. Apparent molar volume

The experimental values of densities of thiamine-HCl having molalities of (0.02, 0.04, 0.06, 0.08 and 0.10) mol kg^{-1} in water and in (0.1, 0.2 and 0.3) mol kg^{-1} aqueous solutions of glucose/lactose, measured at T = (293.15, 298.15, 303.15, 308.15 and 313.15) K are presented in Table 2. Fig. 1 showing a comparison of densities of thiamine-HCl in aqueous medium at T = (298.15 and 308.15) K is found to be in good agreement with the available literature values [7,9,11]. The data at other temperatures could not be found from the literature. Further, a representative 3D-plot of density with temperature and molality of thiamine-HCl in 0.2 mol kg^{-1} aqueous solution of glucose has been exhibited in Fig. 2 which reveals that the density increases with molality of thiamine-HCl but decreases with increasing temperature. These experimental values of densities were used to calculate apparent molar volumes (V_ϕ) using following equation:

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

where m is the molality (mol kg^{-1}) and M is the molar mass (kg mol^{-1}) of solute, ρ_0 and ρ are the densities (kg m^{-3}) of the solvent (water and aqueous solutions of glucose/lactose) and solution (thiamine-HCl + water + glucose/lactose), respectively. The values of V_ϕ, reported in Table 2 reveal that apparent molar volume for thiamine-HCl increase with an increase in molality as well as with increase in temperature. Such trends in apparent molar volumes suggest that the interactions between solute and solvent as well as those between solute-solute or solute-cosolute change with solvent compositions and temperature. However, more clear information regarding solute-solute and solute-solvent interactions may be obtained from limiting apparent molar volumes at infinite dilution.

Table 1
Materials used.

Chemical name	Source	Mass fraction purity	Structure
Thiamine-HCl	Sigma Aldrich, India	>0.990	
D-(+)-Glucose	Sigma Aldrich, India	≥0.995	
α-Lactose monohydrate	Sigma Aldrich, India	>0.990