Food Chemistry 237 (2017) 181–190

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

Solvation behavior and sweetness response of carbohydrates, their derivatives and sugar alcohols in thiamine HCl (vitamin B1) and pyridoxine HCl (vitamin B6) at different temperatures

Parampaul K. Banipal *, Mousmee Sharma, Tarlok S. Banipal

Department of Chemistry, Guru Nanak Dev University, Amritsar 143005, India

ARTICLE INFO

Article history:
Received 4 March 2017
Received in revised form 16 May 2017
Accepted 16 May 2017
Available online 19 May 2017

Chemical compounds studied in this article:
Thiamine hydrochloride (PubChem CID: 6202)
Pyridoxine hydrochloride (PubChem CID: 6019)
(+)-D-Glucose (PubChem CID: 5793)
(+)-Methyl-α-D-glucopyranoside (PubChem CID: 64947)
(+)-D-Xylose (PubChem CID: 135191)
(+)-D-Galactose (PubChem CID: 6036)
Xylitol (PubChem CID: 6912)
Galactitol (PubChem CID: 11850)
(+)-Cellobiose (PubChem CID: 10712)
2-Deoxy-D-Glucose (PubChem CID: 9062)

Keywords:
Solvation
Thiamine HCl
Pyridoxine HCl
Carbohydrate
Sugar alcohol
Standard partial molar volume
Taste quality
Spectroscopic studies

ABSTRACT

Volumetric properties are important tools to study the solvation behavior of solutes and reveal valuable information about solute-solute/cosolute interactions. Therefore, standard partial molar volumes at infinite dilution have been calculated from density measurements for monosaccharides, their methoxy and deoxy derivatives, disaccharides and sugar alcohols in (0.05, 0.15, 0.25 and 0.35) mol kg^{-1} thiamine $HCl_{(aq)}$ and pyridoxine $HCl_{(aq)}$ solutions over temperature range (288.15–318.15) K at pressure, p = 0.1 MPa. The corresponding transfer volumes, expansibilities and apparent massic volumes have been evaluated to examine the solvation behavior and the basic taste quality of studied solutes. UV–Vis absorption study of these solutes has also been carried out in 1.0×10^{-4} mol kg^{-1} thiamine HCl and pyridoxine HCl solutions. Results have been compared with our previously reported studies carried out in L-ascorbic acid (vitamin C). Stereochemical effects on hydration controlled by dominant conformations of studied solutes have also been discussed.

1. Introduction

Sugar alcohols are artificial nutritive sweeteners owing to their desirable properties such as good taste, low calorie content, no tooth decay and widely applied in many other products such as cosmetics, explosives, and plasticizers (Zhu, Ma, & Zhou, 2010). Sugar derivatives are also important to biological systems. One of the most frequently utilized antiglycolytic agent; 2-deoxy-D-glucose, phosphorylated by hexokinase leads to intracellular ATP depletion via the glycolytic pathway. 2-deoxy-D-Glucose has also been considered as a potential anticancer agent (Pelicano, Martin, Xu, & Huang, 2006). A nonmetabolizable sugar, (+)-methyl-α-D-glucopyranoside is known to be accumulated against a concentration gradient by human renal cortical slices (Segal, Genel, Holtzapple, & Rea, 1973). Carbohydrates located at cell surface are receptors to the bioactive structures of enzymes, viruses, antibodies, hormones, etc (Wang, Fu, Guo, & Lin, 2014). Carbohydrates and their derivatives participate in many biological processes, such

* Corresponding author.
E-mail addresses: pkbanipal@yahoo.com (P.K. Banipal), mousmee.sharma90@gmail.com (M. Sharma), tsbanipal@yahoo.com (T.S. Banipal).

http://dx.doi.org/10.1016/j.foodchem.2017.05.078
0308-8146/

as signaling, cell-cell recognition, and molecular and cellular communication due to their conformational flexibility (Banipal, Aggarwal, & Banipal, 2015; Fuchs & Kaatze, 2001). Therefore, their thermodynamic properties along with other bioactive compounds are absolutely of great value.

Thiamine HCl (vitamin B1) and pyridoxine HCl (vitamin B6) are important water-soluble vitamins and play biological roles in the metabolic processes of the carbohydrates in the human body. An accurate estimation of the level of vitamins B1 and B6 is very important in the food as well as in clinical setting (Leporati et al., 2005). The vitamins are reported to reduce the damage by free radicals and aides in preventing degenerative disease. The major biologically active form of thiamine i.e., thiamin diphosphate (TDP), serves as a coenzyme in several enzyme complexes and play important roles in the metabolism of carbohydrates, fats, and alcohol (Buchholz, Drotleff, & Ternes, 2012). Pyridoxine, a precursor of pyridoxal is an important vitamin for the production of RBCs (red blood cells), the cells of the immune system and for maintaining healthy nerve and muscle cells. Pyridoxine HCl is recommended for supplemental use in tuberculosis treatment to prevent isoniazid-induced neuropathy. In addition to medicine, pyridoxine HCl can also be used as food fortification agent or food additive (Han et al., 2016).

The hydration characteristics of carbohydrates have both scientific and practical importance because these are related to their crystallization rate, water sorption, glass transition temperature (T_g) and biopreservation properties (Gharsallaoui, Roge, & Mathlouthi, 2008). These are also involved in the reception of sweetness and environmental stress tolerance. An in-depth understanding of the hydration properties of sugars is important in taste chemoreception mechanism (Aroulmoji, Mathlouthi, Feruglio, Murano, & Grassi, 2012; Banipal, Singh, Aggarwal, & Banipal, 2015). Sugar hydration is influenced by the molecular conformation and the stereochemistry of the solute (Franks, 1985). A systematic study on volumetric and spectroscopic properties for these solutes is needed to understand solute-solute/cosolute interactions. The physico-chemical properties of some vitamins have been reported only in water and in dilute HCl or aqueous NaCl solutions (Ayranci, Sahin, & Ayranci, 2007; Banipal, Singh, Banipal, & Singh, 2013; Dhondge, Deshmukh, & Paliwal, 2013). Recently, we have reported (Banipal, Sharma, & Banipal, 2016a; Banipal et al., 2016b) the volumetric, UV absorption, calorimetric and viscometric studies in order to understand the solvation behavior of monosaccharides, their methoxy and deoxy derivatives, disaccharides and sugar alcohols in L-ascorbic acid$_{(aq)}$ solutions at T = (288.15–318.15) K. To explore the solvation behavior and sweet response, we have carried out the volumetric and spectroscopic studies of these solutes in water and in aqueous (0.05, 0.15, 0.25 and 0.35) mol kg^{-1} thiamine HCl and pyridoxine HCl (cosolutes) solutions at (288.15–318.15) K under atmospheric pressure, p = 0.1 MPa.

2. Materials and methods

2.1. General

The provenances including mass fraction purity, source of procurement and abbreviations of the chemicals used are: (+)-D-xylose (Xyl, ≥99%), (+)-D-galactose (Gal, 98%), (+)-D-glucose (Glc, ≥99%), (+)-methyl-α-D-glucopyranoside (Me-α-Glc, ≥ 99%), sucrose (Suc, ≥ 99%), (+)-cellobiose (Cel, 98%), (+)-maltose monohydrate (Mal, 99%), thiamine hydrochloride (thiamine HCl, ≥99%) and pyridoxine hydrochloride (pyridoxine HCl, ≥99%) {Sigma Chemical Co.}, 2-deoxy-D-glucose (2-de-Glc, 99%), xylitol (Xyol, ≥99%), and galactitol (Gaol, 99%) {Sisco Research Laboratories, India}. The chemicals were used without prior treatment but stored in vacuum desiccator with anhydrous $CaCl_2$ before use. Deionised, doubly distilled and degassed water with specific conductance less than 1.29 × 10^{-4} S m^{-1} was used for the preparation of all the solutions. The solutions were prepared on the mass basis by using Mettler balance having an accuracy of ±0.01 mg.

2.2. Equipments and procedure

2.2.1. Density measurement

The density measurements were carried out by using vibrating-tube digital densimeter (*Model DMA 60/602, Anton Paar, Austria*) at constant temperature (using constant temperature bath, *Model: Julabo F-25*) within ±0.01 K. The calibration of densimeter was done using pure water and dry air and its working was checked by measuring the densities of $NaCl_{(aq)}$ solutions at 298.15 K, which agreed well with the literature values (Zhang & Han, 1996). The standard uncertainty in the densities on an average is ±3.7 × 10^{-6} g cm^{-3}.

2.2.2. UV–Vis absorbance measurement

UV–Visible absorption spectra for varying concentrations of studied solutes in aqueous solutions of thiamine HCl and pyridoxine HCl were recorded on a spectrophotometer (*SHIMADZU UV-1800*) provided with 1.0 cm quartz cells equipped with a Teflon stopper. Baseline correction was applied for each spectrum and the range of λ_{max} = (190–400) nm was surveyed. The concentration of thiamine HCl and pyridoxine HCl was 1.0 × 10^{-4} mol kg^{-1} and the concentrations of solutes were varied in the range (0.00992–0.13430) mol kg^{-1}. The pH of solution was measured using pH meter (*Systronics μ pH System 361*).

3. Results and discussion

3.1. Apparent and partial molar volumes

The density, ρ has been measured for the monosaccharides, their methoxy and deoxy derivatives, disaccharides and sugar alcohols in m_B (molality of thiamine HCl and pyridoxine HCl) = (0.05, 0.15, 0.25 and 0.35) mol kg^{-1} aqueous solutions of thiamine HCl and pyridoxine HCl at (288.15, 298.15, 308.15 and 318.15) K. The apparent molar volumes, $V_{2,\phi}$ for studied solutes have been determined from the experimentally measured density data using the relation:

$$V_{2,\phi} = [M/\rho] - [(\rho - \rho_o)/(m_A \rho \rho_o)] \quad (1)$$

where M and m_A are the molar mass and molality of solute, ρ_o and ρ are the densities of the pure H_2O or mixed solvent (H_2O + cosolute) and ternary solution (solute + H_2O + cosolute), respectively. The densities of solutions increase with increase in molalities of solute as well as cosolute (thiamine HCl and pyridoxine HCl), but decrease with rise of temperature in all cases. 3-D plot of density, ρ versus m_A, molality of (+)-methyl-α-D-glucopyranoside in m_B = 0.15 mol kg^{-1} thiamine $HCl_{(aq)}$ solutions at T = (288.15–318.15) K is given in Fig. 1. The $V_{2,\phi}$ values for the anhydrous (+)-maltose have been calculated by applying the molality correction to its hydrate i.e., (+)-maltose monohydrate. The density and $V_{2,\phi}$ data are given as supporting information in Table S1. The data reveal that $V_{2,\phi}$ values for studied solutes increase with increase in cosolute concentration and temperature. Furthermore, $V_{2,\phi}$ parameter suggests that an increase in molar mass of the solute has more probability of contracting cosolute molecules, which in turn may enhance the solute-cosolute interactions (Banipal, Kaur, Kaur, Gupta, & Banipal, 2015). The structures of studied carbohydrates, their derivatives, sugar alcohols and vitamins (B1 and B6) are given in Fig. 2.