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Intermolecular hydrogen bonding formation in aqueous D-Mannitol

O.P.Chimankar[1], Ranjeeta Shriwas[1] and V.A.Tabhane[2]

[1]Department of Physics, RTM Nagpur University, Campus, Nagpur
[2]Department of Physics, Pune University, Pune

ABSTRACT

The density and ultrasonic velocity measurements were carried out in aqueous solutions of D-mannitol in the concentration range of 0.1 to1.0 M and temperature between 303.15K to 323.15K.. The thermoacoustical parameters viz. adiabatic compressibility, free volume, internal pressure and Moelwyn-Hughes parameter have been computed from the experimental parameters shows nonlinear increase or decrease with various concentrations and temperatures. These parameters were interpreted as due to the formation of intermolecular hydrogen bonding between the hydroxyl groups of D-mannitol and water molecules.

Keywords: Hydrogen bonding, Molecular association, Moelwyn- Hughes parameter, Internal Pressure

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INTRODUCTION

Carbohydrates play an important role in animal and plant life. Understanding the behavior of aqueous carbohydrate solution is of almost important in biology, medicine and understanding the taste quality exhibited by them [1]. The study of D-mannitol in water environment is of fundamental importance for biological reasons. The polyhydroxy compounds help in stabilizing the native conformation of globular proteins [2,3]. In proteins and enzymes, sugars and polyols are known stabilizing agents in their native state and their strong interaction with water [4,5]. The various thermodynamics and spectroscopic studies have been shown that the hydration of saccharides depends upon the number of hydroxyl groups.

Apparent molar volumes and apparent specific volumes reflect the state of hydration of the molecules and thus their extent of interaction with water structure [6-8]. In this paper, an attempt has been made to understand the molecular interaction of D-mannitol with water by evaluating various acoustic parameters based on the ultrasonic velocity measurements in aqueous solutions of D-mannitol at various concentrations and temperatures.

MATERIALS AND METHODS

Sample preparation and experimental techniques

Aqueous solutions of D-mannitol in the concentration range of 0.1 to 1.0 m are prepared by dissolving known amounts of D-mannitol in the double distilled water. The derived properties in this work, over the entire range of mass concentration in aqueous solutions of D-mannitol in the temperature range of 303.15K-323.15K at intervals of 5K. In these systems, the above properties are more studied to examine the effect of temperature.

Using the measured data, the acoustical parameters such as adiabatic compressibility (β_a) fractional free volume (V_f), internal pressure (Pi) and Moelwyn-Hughes parameter (C_1) were calculated using the following standard expressions.

Adiabatic compressibility β_a ($N^{-1}m^2$),

$$\beta_a = 1/u^2\rho \quad (1)$$

Where, u = sound velocity of solution (m/s) and

ρ = density of solution at the same temperature (Kg/m^3)

Free volume can be expressed as

$$V_f = (V/u^3)\,(\gamma RT/M)^{3/2} \quad (2)$$

Where, V = is the Molar volume, M = Molecular weight

T = is the absolute temperature, R = Rao constant

γ = is the ratio of specific heats = 1.5

Internal pressure can also be expressed as,

$$Pi = \rho u^2 / (B/A + 1) \quad (3)$$

Where, $B/A = C_1-1$ is the Bayer's nonlinearity parameters

Moelwyn-Hughes parameter (C_1) can be written as,

$$C_1 = [13/3+ (\alpha T)^{-1} + 4/3\ \alpha T] \quad (4)$$

Where, $\alpha = (1/\rho)\,(d\rho/dt)$ is the volume expansivity

Gruneisen parameter $\Gamma= (C_1-1)/2$ (5)

RESULTS AND DISCUSSION

Number of studies has been focused on the ultrasonic properties of biomaterial solution [3-10]. The object of those studies is to identify the molecular interaction between biomaterial and solvent. Recently the ultrasonic study on the solution of D-mannitol provides sample evidence for intermolecular force operating between D-mannitol and water [3]. The present study was taken under acoustical behavior of D-mannitol at several concentrations and temperatures.

The necessary data of ultrasonic velocity and density in aqueous D-mannitol at various concentrations and temperatures were taken by using Pulse echo overlap and pyknometer method. The related acoustical parameter i.e. adiabatic compressibility (β_a) fractional free volume (V_f), internal pressure (Pi) and Moelwyn-Hughes parameter (C_1) are computed by given formulae and shown graphical representation in figure 1 to 4 at various concentrations and temperatures.

In ultrasonic velocity is found to increase with the increase in mannitol concentration. The increase in ultrasonic velocity in any solution indicates the maximum association among the molecules of solution. The maximum association is due to the hydrogen bonding between the solute and solvent molecules [6-10]. The conductivity studies of sucrose solutions and acoustical properties of fructose and maltose in water and in aqueous NH_4Cl solutions also confirm the formations of hydrogen bonds between the solute and water molecules [1, 2].

Figure 1 shows that, adiabatic compressibility is decrease with the increase in temperature and D-mannitol concentrations. This confirms the presence of solute-solvent interactions through dipole-dipole interactions of the-OH groups of mannitol with the surrounding water molecules [3].

Figure 2 and 3 shows the free volume (V_f) decrease and internal pressure with is increasing temperature and concentration. It shows reverse trend, which indicates molecular association between D-mannitol and water molecules. The stronger intermolecular force due to thermal agitation of molecule in aqueous mannitol.

Moelwyn-Hughes Parameter in figure 4 increase with increase in temperatures and concentrations. These indicate loosing of intermolecular force due to thermal agitation of the molecule in the aqueous mannitol solutions at higher temperature.The similar variations are also found in Bayer's nonlinearity parameter and Gruneisen parameter (not shown). These calculated values with increasing mannitol concentration also strongly support the association.

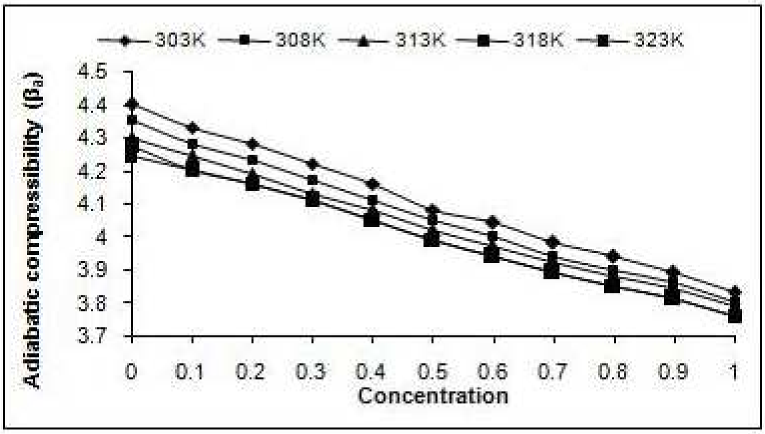

Figure.1:Variation of adiabatic compressibility with concentration and tempertures

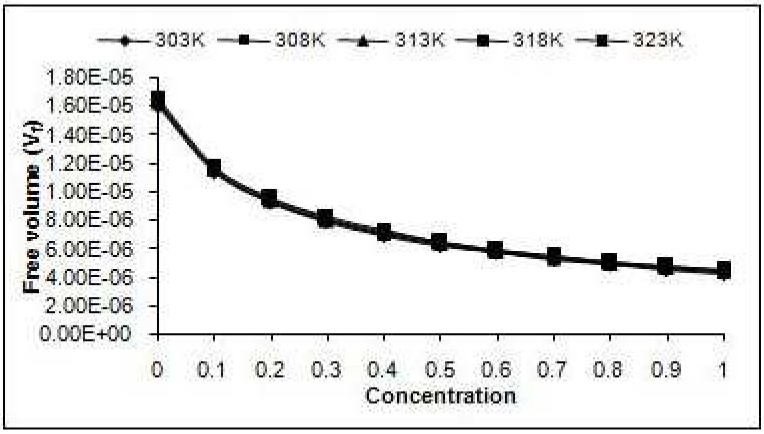

Figure2: Variation of Free Volume with concentrations and temperatures

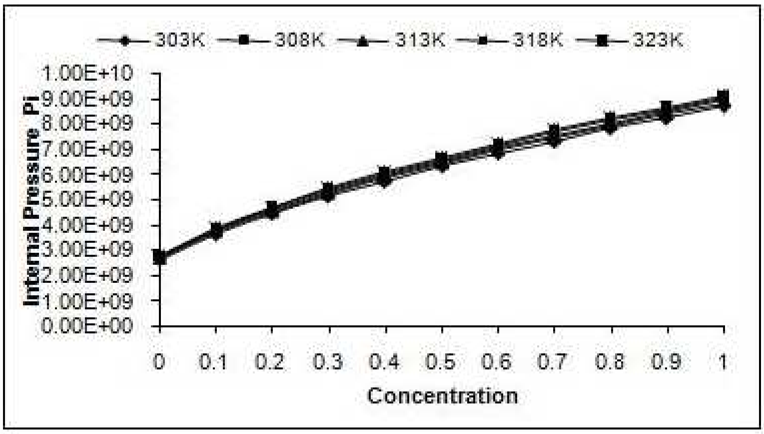

Figure 3: Variation of Internal Pressure with concentrations and temperatures

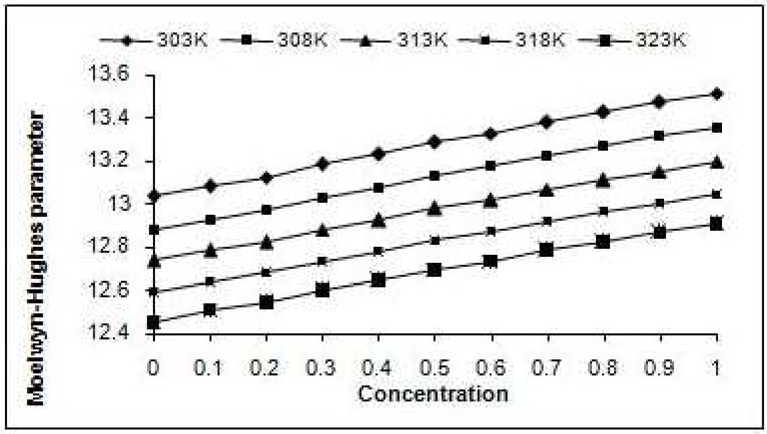

Figure 4: Variation of Moelwyn Hughes parameter with concentrations and temperatures

CONCLUSION

The molecular association between D-mannitol and water molecules arises due to the hydrogen bonding formation. D-mannitol shows hydrophilic nature with water molecules. Hence D-mannitol is playing a very important role in food, medical and pharmaceutical industry as water contains product.

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