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Thermodynamic parameters and ultrasonic studies of intermolecular interactions in some carbohydrates (Dextrose, Fructose and Inositol) at 298.15 k.

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ABSTRACT

Ultrasonic velocity, density and viscosity have been measured experimentally of aqueous solution of dextrose, fructose and inositol at 298.15 K over the entire composition range. The useful thermodynamic parameters like Gibb's free energy (ΔG), enthalpy (ΔH) and entropy (ΔS) etc. have been worked out. In the light of these parameters molecular interactions among the liquid mixture have been discussed.

Keywords: Ultrasonic velocity, Inositol, Gibb's free energy, Enthalpy, Entropy.

INTRODUCTION

The study of inter molecular interactions play an important role in the development of molecular sciences. A wide study has been made on the molecular interaction in liquid system by various spectroscopic methods [1]. Ultrasonic investigation provides wide application in characterizing thermodynamic and physiochemical behavior of liquid mixture [2]. These acoustical parameters grant qualitative information about physical nature and strength of molecular interaction in liquid mixtures. During the last two decades the ultrasonic study of the carbohydrates in aqueous electrolytic medium, has gained much importance in assessing the nature of molecular interaction present in the mixture. The study of the carbohydrates or saccharides has become a subjects of growing interest because of multidimensional, physical, biochemical and scientifically useful molecules [3-6]. Due to composite molecular structure of polysaccharides, straight study is difficult. Therefore, the suseful approach is to study simpler form compounds, such as Dextrose, Fructose and Inositol which are building blocks of polysaccharides. Most of the studies on carbohydrates have been carried out in pure and mixed solvent [7-9].

Most of the studies have been done concerning to the intermolecular interaction of carbohydrates in electrolytes and non electrolytes medium. But in our present work, not only considered the molecular interaction but also the stereo specific relationships among them. These are very important biological molecules.

Carbohydrates displayed on the surface of cells play critical roles in cell-cell recognition, adhesion, signaling between cells, and as markers for disease progression. Neural cells use carbohydrates to facilitate development and regeneration [10]; cancer cell progression is often characterized by increased carbohydrate-dependent cell adhesion and the enhanced display of carbohydrates on the cell surface [11]; viruses recognize carbohydrates to gain entry into host cells [12]; and bacteria bind to carbohydrates for host cell adhesion[13]. Recognition of the specific saccharides involved in these processes is important to better understand cell-cell recognition at the molecular level and to assist the design of therapeutics and diagnostic tools.

Why glucose is so widely used than the other monosaccharides such as fructose in organisms, it is not clearly understood. One reason might be that glucose has a lower tendency than other hexose sugars to react non-

specifically with the amino groups of proteins. This reaction - (glycation) - reduces or destroys the function of many enzymes. The low rate of glycation is due to glucose's preference for the less reactive cyclic isomer. However, many of the long-term complications of diabetes are probably due to the glycation of proteins or lipids[14]. In contrast, enzyme-regulated addition of glucose to proteins by glycosylation is often essential to their function. Another reason as to why glucose is the most common sugar is that it is the most conformationally stable compared to other possibilities.When glucose is low, psychological processes requiring mental effort (e.g., self-control, effortful decision-making) are impaired [15].

Apple and pear juices are of particular interest to pediatricians because the high concentrations of free fructose in these juices can cause diarrhea in children. The cells (enterocytes) that line children's small intestines have less affinity for fructose absorption than for glucose and sucrose. Unabsorbed fructose creates higher osmolarity in the small intestine, which draws water into the gastrointestinal tract, resulting in osmotic diarrhea[16].

Chemistry and biology of *myo*-inositol derivatives has been investigated widely in the recent past due to the association of phosphoinositols in cellular signal transduction mechanisms[17] and anchoring of certain proteins to cell membranes[18]. Although a bewildering array of *myo*-inositol phosphates and their lipid derivatives have been identified and / or isolated from plant as well as animal sources, the biological roles played by many of them is not yet clearly understood. However, receptors and effectors involved in various stages of phosphoinositol based signal transduction pathways remain potential targets for pharmacological intervention in states of disease[19].These developments in biology and medicine have necessitated the efficient synthesis of naturally occurring phosphoinositols and their synthetic analogs.

The studies of these molecules in aqueous medium are very important for biomolecular recognition and medicinal use.

MATERIALS AND METHODS

Experimental

The solutions of Dextrose, Fructose and Inositol were prepared by dilution method. All the chemicals are of AR grades of 99.99 % purity. Composition range of each substance is from 0.1 M to 0.9M.

The ultrasonic velocity in the liquid mixtures have been measured by means of ultrasonic interferometer (Mittal type : Model: M-83) functioning at frequency 2MHz with an overall accuracy of ±0.1 m/s , an electronically digital operate constant temperature water bath has been used to flow water through the double walled measuring cell, made up of a steel containing the experimental solution at the preferred temperature. For weighing, an electronic digital balance having an accuracy of ±0.1 mg was used. An Ostwald's viscometer was used for the measurement of viscosity of liquid mixtures with an accuracy of 0.0001Nsm2. The viscometer was calibrated before used. Time flow of water and liquid solutions were measured. Densities were determined using specific gravity bottle by relative measurement method with accuracy of ±0.1 $kg.m^{-3.}$

RESULTS AND DISCUSSION

The experimental parameters such as density, ultrasonic velocity and viscosity are shown in tables 1, 2 &3 for Dextrose, fructose and Inositol respectively.

From these parameters, Gibb's free energy (ΔG), enthalpy (ΔH) and entropy (ΔS) are worked out and correlation of intermolecular interactions was established by plotting graphs.

Relaxation time is obtained using equation;

$$\tau = \left(\frac{4}{3}\right) \eta \beta_a \text{ sec} \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Internal pressure (π_i) can be calculated by expression.

$$\pi_i = bRT\,(K\eta/u)^{1/2}(\rho^{2/3}/M)^{7/6}\ Nm^{-2} \ldots\ldots\ldots\ldots\ldots(2)$$

Where R is the gas constant, M is the effective molecular weight, ρ is the density, u is the velocity of sound, T is the temperature, η is the viscosity and K is the temperature independent constant.

Gibb's free energy(ΔG **)**can be calculated from the following relation:

$$\Delta G = KT \log (KT\tau/ h) \quad \text{…… (3)}$$

Where, τ is relaxation time, K is Boltzmann constant, T is absolute temperature and h is Plank's constant[20].

Enthalpy(ΔH) of solutions were worked out from the following relation[21]:

$$\Delta H = Li/Meff \quad \text{…….. (4)}$$

Where, Li is latent heat of vaporization and Meff is effective molar mass of solution.

Entropy(ΔS) of solution can be calculated from the following relation[22]:

$$\Delta S = \Delta H - \Delta G/T \quad \text{……(5)}$$

Where, T is absolute temperature in Kelvin.

Table-1. Values of density(ρ), Viscosity(η),Ultrasonic velocity(u), Gibb's Free energy , Enthalpy and Entropy at 298.15 K of aqueous solution of Dextrose.

Conc.(molar)	P (Kgm^{-3})	U (ms^{-1})	η (NSm^{-2})	ΔG $*10^{-21}$ $KJmol^{-1}$	ΔHi $*10^{6}$ $KJmol^{-1}$	ΔS $KJmol^{-1}K^{-1}$
0.9	1058.1	1560	1.003	4.93944	1.887	6329.06
0.8	1049.9	1556	0.995	4.84628	1.932	6482.24
0.7	1041.8	1557	0.945	4.66059	1.964	6588.09
0.6	1034.4	1551	0.883	4.44233	1.985	6660.85
0.5	1025	1542.4	0.850	4.36887	2.044	6855.80
0.4	1019.5	1538.8	0.818	4.25227	2.100	7046.38
0.3	1012.9	1532	0.789	4.16685	2.168	7273.12
0.2	1007.3	1529.6	0.768	4.09152	2.248	7542.12
0.1	1001.9	1524	0.743	4.00759	2.331	7820.46
0.0	997.4	1512.8	0.713	3.91717	2.416	8106.37

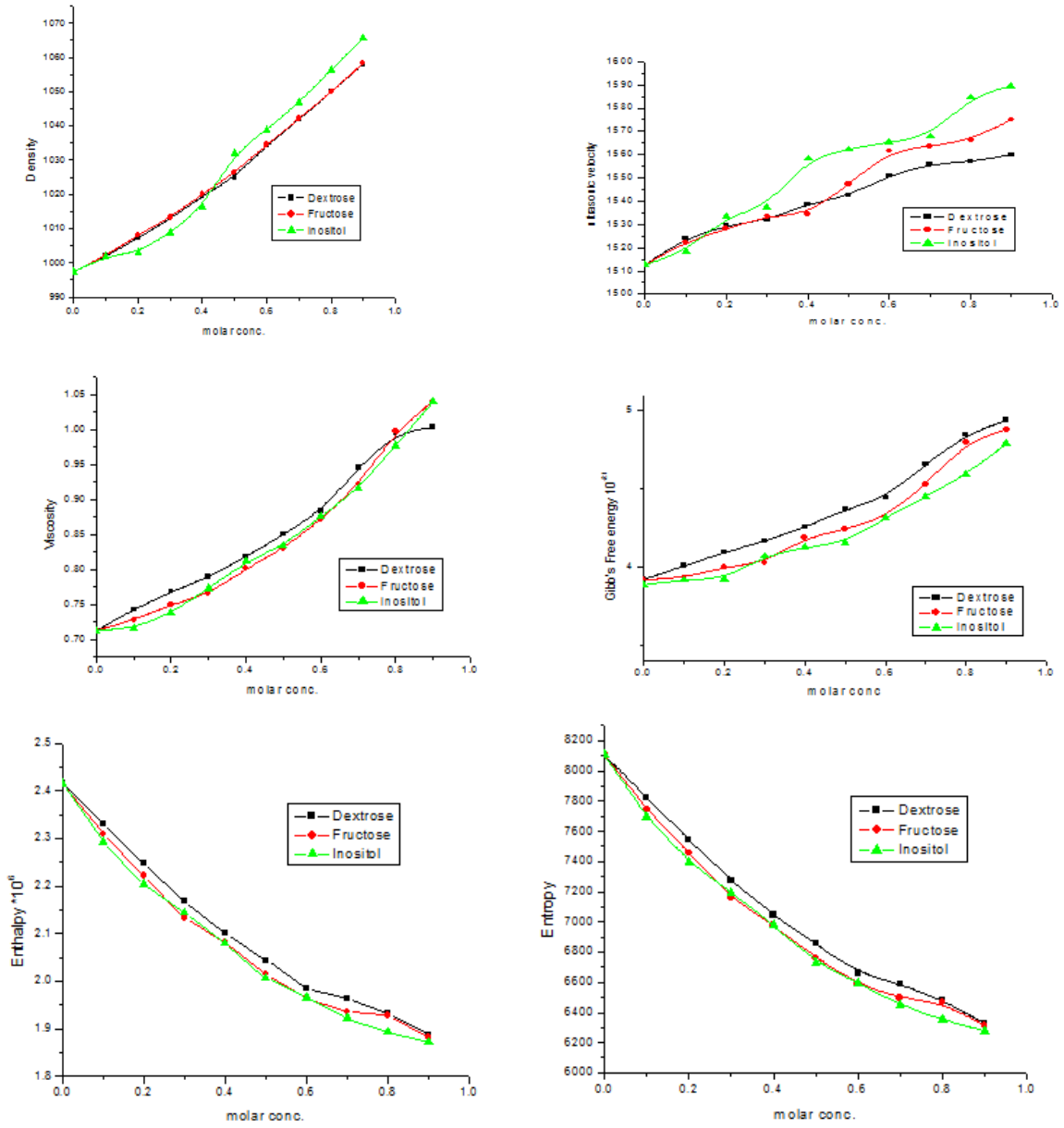
Table-2. Values of density(ρ), Viscosity(η),Ultrasonic velocity(u), Gibb's Free energy , Enthalpy and Entropy at 298.15 K of aqueous solution of Fructose

Conc.(molar)	P (Kgm^{-3})	U (ms^{-1})	η (NSm^{-2})	ΔG $*10^{-21}$ $KJmol^{-1}$	ΔHi $*10^{6}$ $KJmol^{-1}$	ΔS $KJmol^{-1}K^{-1}$
0.9	1058.3	1575	1.04	4.879	1.882	6313.70
0.8	1050.0	1566.4	0.997	4.799	1.928	6466.97
0.7	1042.1	1561.6	0.921	4.529	1.936	6493.69
0.6	1034.5	1563.6	0.871	4.318	1.964	6588.51
0.5	1026.4	1547.2	0.830	4.239	2.015	6761.07
0.4	1020.1	1534.4	0.801	4.187	2.081	6981.62
0.3	1013.3	1533.6	0.765	4.029	2.133	7156.97
0.2	1008.2	1528.2	0.750	3.998	2.222	7454.90
0.1	1002.1	1522.4	0.728	3.931	2.309	7744.67
0.0	997.4	1512.8	0.713	3.917	2.416	8106.37

Table-3. Values of density(ρ), Viscosity(η),Ultrasonic velocity(u), Gibb's Free energy , Enthalpy and Entropy at 298.15 K of aqueous solution of Inositol

Conc.(molar)	P (Kgm^{-3})	U (ms^{-1})	η (NSm^{-2})	ΔG $*10^{-21}$ $KJmol^{-1}$	ΔHi $*10^{6}$ $KJmol^{-1}$	ΔS $KJmol^{-1}K^{-1}$
0.9	1065.6	1589.6	1.04	4.7874	1.872	6279.33
0.8	1056.4	1584.8	0.977	4.5946	1.893	6351.63
0.7	1046.8	1568	0.915	4.4500	1.922	6449.60
0.6	1038.9	1565.4	0.876	4.3155	1.966	6594.26
0.5	1032.0	1562.4	0.834	4.1565	2.007	6732.07
0.4	1016.3	1558.4	0.811	4.1256	2.080	6979.27
0.3	1008.7	1537.6	0.773	4.0695	2.145	7195.84
0.2	1003.1	1533.6	0.738	3.9231	2.204	7393.99
0.1	1001.9	1518.4	0.716	3.8855	2.293	7691.20
0.0	997.4	1512.8	0.713	3.9171	2.416	8106.37

Graph 1-3 of Ultrasonic velocity (U), Density (ρ) and Viscosity (η), and Graph4-6 of Gibb's Free energy (ΔG) , Enthalpy(ΔH) and Entropy(ΔS) of Dextrose, Fructose and Inositol.



A measure of how strongly molecules are held in liquid mixtures is their Gibb's free energy, enthalpy and entropy. These are considered to be very important thermodynamic parameters. These parameters give information about how closed the liquid molecules are held, freedom of motion, the amount of empty space in liquid mixture, bulk properties of mixture (melting point, boiling point, solubility and fractional distillation),what types of forces (dipole-dipole, ion-dipole, ion-induced dipole and dipole-induced dipole) in liquid molecules exit. Of these some parameters are directly and some are inversely related to the strength of intermolecular forces that exit in liquid mixtures. Intermolecular forces may be long range or short range forces. Long range forces are dispersion forces and electrostatic induction. They occur when molecules come close together causing a significant overlap of electron density having a specific geometry.

Graph1-3 shows the plot of ultrasonic velocity (U), density (ρ) and viscosity (η) versus concentration at 2MHz and 298.15K temperature of dextrose, fructose and inositol. It is observed that all these parameters increased with increase in concentration of monosaccharide's in water indicating strong hydration of glucose, fructose and inositol in component molecules. This behavior suggests the formation of more compact structure, possible due to dipole-dipole interaction (hydrogen bonding) at the sites on the hydroxyl group (OH) of sugars and water molecules. The

association in constituent molecules may involve due to hydrogen bonding or dipole-dipole interaction among the constituent molecules. All these process may lead to strong solute-solvent interactions

Graph4 shows the plot of Gibb's free energy versus concentration at 2MHz and 298.15K temperature of dextrose, fructose and inositol. It is observed that Gibb's free energy (ΔG) increases with increase in concentration. This indicates that solution is highly ordered due to strong association among the solute and solvent molecules. This also indicates the strong hydration and low mobility of solvent molecules.

Graph5-6 show the plot of enthalpy (ΔH) and entropy (ΔS) versus concentration at 2MHz and 298.15K temperature of dextrose, fructose and inositol. It is observed that these parameters decreased with increase in concentration suggest that solute and solvent molecules are strongly associated. Lower the values of enthalpy more would be the salvation and strong will be the molecular interaction among the constituent molecules.

Entropy measures the freedom of the molecules in the given medium. Higher the freedom lower will be the molecular association and vice-versa. In the present work, at higher concentration entropy is lower suggested low freedom of molecules and hence strong molecular interaction. It is known that the hydration of carbohydrates depends on the percentage of axial and equatorial hydroxyl groups. It is more favorable when the hydroxyl group is at the equatorial position [23].It seems that hydration of equatorial –OH groups is more compact having lower entropy compared with water at normal temperature. The water around axial –OH groups seems to be less compact hence should have higher entropy. Glucose has more percentage of equatorial –OH group, would be strongly hydrated as compared to fructose and inositol. But result shows that the trend of hydration is dextrose<fructose<inositol. This can be explained that glucose is present as a pyranose ring and fructose as furanose ring which has also five –OH groups but out of these five, two are attached to $–CH_2$ groups and not to the ring. It is known that the interactions between open chain aliphatic –OH groups and water are more extensive than cyclic compounds with water[24]. Hence fructose is slightly more hydrated than dextrose. Inositol has same percentage of equatorial –OH groups but one –OH group is more than dextrose and fructose and hence lower values of entropy, suggest strong hydration.

CONCLUSION

Intermolecular interactions of sugars with water depend on the position (equatorial or axial) of –OH groups, cyclic and acyclic nature –OH groups and number of –OH groups in the molecules. It is also conclude that specific configuration of sugar molecules play important role in hydration processes as presented in present work on basis of useful thermodynamic parameters.

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