Studies on adiabatic compressibilities of some saccharides in aqueous magnesium chloride solutions over temperature range (288.15 to 318.15) K

Amanpreet K. Hundal*,

Department of Chemistry, Guru Nanak Dev University,
Amritsar 143 005, India
E-mail : amanchahal.chem@gmail.com

Parampaul K. Banipal, Tarlok S. Banipal

Department of Chemistry, Guru Nanak Dev University,
Amritsar 143 005, India
E-mail : pkbanipal@yahool.com

Abstract—**Apparent molar adiabatic compressibilities, $K^0_{s,2,\phi}$ at inifinite dilution of various mono-, di-, tri-saccharides and methylglycosides have been determined in water and in aqueous solutions of magnesium chloride (0.5, 1.0, 2.0 and 3.0) mol · kg^{-1} at temperatures T = (288.15, 298.15, 308.15 and 318.15)K from sound velocities employing multifrequency ultrasonic interferometer. Partial molar adiabatic compressibilities at infinite dilution, $K^0_{s,2}$ were extrapolated from $K_{s,2,\phi}$ data and used to calculate transfer compressibilities from water to aqueous magnesium chloride solutions. The $\Delta_t K^0_{s,2}$ values are positive, and generally there is an increase in $\Delta_t K^0_{s,2}$ values with concentration of a cosolute at all the temperatures studied. Furthermore, the $\Delta_t K^0_{s,2}$ values decrease with temperature. The pair, K_{AB} and triplet, K_{ABB} interaction coefficients, hydration number, n_H have been calculated. The magnitudes of n_H values are less in aqueous solutions of potassium chloride as compared to those in water and decrease with the increase in concentration of magnesium chloride. This shows that the cosolute has dehydration effects on the saccharides. These parameters have been discussed in terms of solute-cosolute interactions.**

Keywords: Saccharides, Methylglycosides, magnesium chloride, Partial molar adiabatic compressibities, Interaction coefficients

I.   INTRODUCTOIN

Saccharides and their derivatives are widely distributed in various forms of life as essential moieties of glycoproteins, glycolipids, nucleic acids and polysaccharides. These are found with an enormous range of complexity, from simple mono- to mega-dalton polysaccharide structures. Because of conformational flexibility, saccharides play significant roles in many biological processes such as signaling, cell-cell recognition, molecular and cellular communication [1-4]. To understand mechanisms of biological processes, low molecular model compounds (e.g. alcohols, saccharides, peptides, nucleic acid bases, nucleosides and nucleotides) have been studied due to the complexities of biomolecules. Saccharides are important compounds due to their hydrophilic hydroxy (–OH) rich periphery, coordinating ability, homochirality, stereospecificity, etc. Saccharides with their well known stereochemistry are logical choices in stereo-selective reactions for the synthesis of biologically active target molecules [5-6]. The hydration characteristics of saccharides in aqueous solutions are of direct relevance for understanding the role of glycoproteins and glycolipids in molecular recognition [7-11].The saccharide components of cell membranes are the receptors of biologically active compounds (enzymes, drugs) etc. Saccharides consisting of an aliphatic moiety and polar –OH groups are appropriate models for studying hydration properties of proteins and nucleic acids. However, the understanding of the relationship between saccharide structure and their biological function is still far behind that of proteins and nucleic acids [2,12]. Thermodynamic and transport properties are very useful in the study of hydration behaviour of saccharides [3,15-22]. In continuation of our volumetric studies [23] on saccharides in aqueous solutions of magnesium chloride , we report here systematically the compressibilities, $K^0_{s,2}$ for seventeen mono-, di-, and tri-saccharides and methylglycosides in water and in (0.5, 1.0, 2.0, and 3.0) mol · kg^{-1} aqueous magnesium chloride (MgCl$_2$) solutions at different temperatures, T = (288.15, 298.15, 308.15 and 318.15) K . Adiabatic compressibilities of transfer, $\Delta_t K^0_{s,2}$, from water to aqueous solutions of MgCl$_2$ (the co-solute) and pair and higher order interaction coefficients (η_{AB}, η_{ABB}) have been calculated. . These parameters have been utilized to understand various mixing effects due to the interactions between saccharide/ methylglycoside (solute) and magnesium chloride (co-solute) in aqueous solutions.

II.   MATERIALS AND EXPERIMENTAL METHOD

All the materials used in the present work are the same as reported earlier [13]. The sound velocity, u was determined using Multifrequency Ultrasonic Interferometer (*Model: M-82, Mittal Enterprises, India*) which is a direct and simple device for the measurement of the sound velocities of the liquids with a high degree of accuracy. . The temperature of the water thermostat was controlled within ± 0.01 K. The uncertainties in sound velocities were ± 0.5 ms^{-1}, while these were precise within ± 0.1 ms^{-1}. The measured value for u in water at 298.15 K (1496.74 ms^{-1}) agrees well with the literature [9-10] value (1496.69 ms^{-1}).

All the solutions were prepared freshly by mass using a Mettler balance with a precision of ±0.01 mg in double distilled deionised and degassed water. The uncertainty in the molality of solutions is of the order of ± 3 x 10^{-6} mol

III.   RESULTS and discussion

The adiabatic compressibilities, $K_{s,2,\phi}$ of the various mono-, di-, tri-saccharides and methylglycosides studied in water and in m_B=(0.5, 1.0, 2.0, and 3.0) mol · kg^{-1} aqueous solutions of MgCl$_2$ at T = (288.15, 298.15, 308.15 and 318.15) K were calculated from the adiabatic compressibility and density data using the following relation:

$$K_{s,2,\phi} = \frac{K_s M}{d} - \frac{K^0_s d - K_s d_0}{m d d_0} \qquad (1)$$

where M is the molar mass, m is the molality of saccharides, d, d_0 and K_s, K^0_s are the densities and adiabatic compressibilities of solution and solvent, respectively. The adiabatic compressibilities were calculated from the sound velocities and densities as follows:

$$K_s = \frac{1}{u^2 d} \qquad (2)$$

where u is the sound velocity.

The uncertainty in the determination of $K_{s,2,\phi}$ because of the measurements of various quantities range from 0.40×10^{-15} to 0.22×10^{-15} m^3 mol^{-1} Pa^{-1} for the lower ($m \leq 0.05$ mol kg^{-1}) and higher concentration range.

At infinite dilution, the apparent molar adiabatic compressibility becomes equal to the partial molar adiabatic compressibility, $K^0_{s,2}$ ($K_{s,2,\phi} = K^0_{s,2}$). The $K^0_{s,2}$ values have been calculated by least-squares fitting of the following equation to the corresponding data as:

$$K_{s,2,\phi} = K^0_{s,2} + S_K m \qquad (3)$$

where, S_K is the experimental slope. The $K^0_{s,2}$ values along with their standard deviations are summarized in Table 1

TABLE 2. PARTIAL MOLAR ADIABATIC COMPRESSIBILITIES, K0s,2, AT INFINITE DILUTION OF VARIOUS SACCHARIDES IN WATER AND IN AQUEOUS SOLUTIONS OF MgCL2 OVER TEMPERATURE RANGE (288.15 TO 318.15)K

$^a m_B/$ (mol kg^{-1})	$K^0_{s,2} \times 10^{15}$			
	T/(K)			
	288.15	298.15	308.15	318.15
D-(+)-Xylose				
0.0	-21.35±0.01	-13.11± 0.01	-11.64±0.002	-10.78±0.001
0.5	-18.54±0.02	-10.80±0.04	-9.63±0.02	-8.85±0.03
1.0	-13.19±0.03	-5.57±0.02	-4.48±0.02	-3.84±0.02
2.0	-10.52±0.04	-2.73±0.02	-1.79±0.03	-1.57±0.01
3.0	-8.24±0.02	-0.98±0.02	-0.27±0.01	-0.79±0.01
D-(–)- Arabinose				
0.0	-28.47 ±0.02	-21.80± 0.01	-13.64 ± 0.04	-12.27± 0.01
0.5	-22.71±0.03	-16.85±0.04	-9.13±0.02	-8.07±0.01
1.0	-18.99±0.04	-12.84±0.01	-4.96±0.03	-3.99±0.05
2.0	-16.11±0.05	-10.25±0.01	-3.17±0.01	-2.60±0.01
3.0	-14.82±0.02	-9.13±0.01	-1.93±0.01	-1.26±0.01
D-(–)-Ribose				
0.0	-14.24± 0.01	-13.10± 0.0001	-12.09± 0.001	-11.20± 0.001
0.5	-7.95±0.03	-6.76±0.004	-5.86±0.02	-5.06±0.02
1.0	-3.49±0.02	-3.15±0.03	-2.22±0.01	-2.15±0.01
2.0	-1.11± 0.02	-0.96±0.03	-0.75±0.01	-0.46±0.01
3.0	-0.31±0.02	-0.33±0.03	-0.10±0.004	-0.57±0.01
D-(+)-Mannose				
0.0	-24.22±0.04	-15.88± 0.03	-14.14± 0.002	-13.65± 0.0001
0.5	-17.21±0.01	-9.38±0.01	-7.75±0.02	-7.36±0.02
1.0	-13.25±0.02	-5.76±0.03	-4.43±0.01	-4.26±0.01
2.0	-10.99±0.02	-3.58±0.04	-2.53±0.004	-2.68±0.002
3.0	-10.07±0.02	-2.58±0.03	-1.85±0.02	-2.16±0.01
D-(–)-Fructose				
0.0	-23.83±0.001	-21.11± 0.02	-20.80± 0.01	-19.30 ±0.02
0.5	-16.72±0.01	-14.30±0.01	-14.19±0.02	-12.78±0.01
1.0	-12.62±0.01	-10.52±0.01	-10.28±0.01	-10.16±0.01
2.0	-10.50±0.02	-8.82±0.01	-8.43±0.01	-8.26±0.03
3.0	-9.56±0.02	-7.50±0.04	-8.11±0.02	-7.77±0.05
D-(+)-Galactose				
0.0	-22.21±0.001	-20.89± 0.001	-20.56± 0.001	-18.92± 0.01
0.5	-14.44±0.02	-13.82±0.02	-13.52±0.004	-11.94±0.004
1.0	-10.30±0.003	-9.41±0.01	-9.31±0.01	-8.31±0.01
2.0	-9.00±0.003	-8.38±0.001	-8.27±0.01	-7.91±0.004
3.0	-7.52±0.01	-7.06±0.02	-7.03±0.002	-6.55±0.02
D-(+)-Glucose				
0.0	-29.86±0.01	-19.04± 0.01	-12.85± 0.03	-12.09± 0.02
0.5	-22.22±0.04	-12.64±0.06	-5.97±0.03	-5.11±0.02
1.0	-17.99±0.02	-8.77±0.04	-2.82±0.01	-2.48±0.01
2.0	-16.28±0.02	-7.26±0.02	-2.30±0.01	-1.95±0.01
3.0	-15.29±0.02	-5.92±0.05	-0.14±0.01	-0.30±0.01
D-(+)-Melibiose				
0.0	-39.11±0.02	-31.33± 0.01	-29.40± 0.01	-28.99±0.0001
0.5	-31.22±0.02	-24.22±0.04	-22.32±0.02	-22.05±0.02
1.0	-27.42±0.02	-20.40±0.01	-19.47±0.01	-19.31±0.01
2.0	-24.64±0.02	-17.56±0.01	-16.77±0.03	16.16±0.003
3.0	-23.84±0.02	-16.96±0.04	-15.82±0.03	-15.51±0.02
D-(+)-Cellobiose				
0.0	-33.89±0.01	-25.60± 0.10	-24.64± 0.02	-21.93± 0.02
0.5	-18.46±0.02	-17.61±0.02	-17.11±0.04	-14.40±0.02
1.0	-14.34±0.02	-14.09±0.003	-14.39±0.07	-11.82±0.05
2.0	-11.16±0.01	-11.43±0.01	-11.41±0.02	-9.42±0.01
3.0	-9.62±0.004	-9.43±0.02	-9.17±0.01	-7.20±0.02
D-(+)-Maltose monohydrate				
0.0	-31.67± 0.01	-23.29± 0.01	-21.87±0.01	-20.93± 0.001
0.5	-21.65± 0.02	-13.77±0.01	-13.02±0.03	-12.48±0.01
1.0	-15.93±0.01	-8.70±0.01	-8.12±0.03	-8.02±0.01
2.0	-8.90±0.02	-4.00±0.01	-3.90±0.01	-5.53±0.02
3.0	-6.49±0.01	-3.22±0.03	-3.10±0.04	-4.46±0.03
Sucrose				
0.0	-27.45± 0.01	-17.51± 0.02	-16.37 ±0.01	-15.67 ±0.03
0.5	-19.30±0.01	-9.49±0.03	-8.56±0.03	-8.06±0.03
1.0	-14.42±0.01	-5.38±0.01	-5.29±0.01	-5.19±0.02
2.0	-11.02 ±0.03	-2.43±0.01	-2.06±0.02	-2.04±0.02
3.0	-9.52±0.01	-0.54±0.02	-0.38±0.01	-0.28±0.004
D-(+)-Lactose monohydrate				
0.0	-38.79± 0.01	-30.60± 0.02	-29.04 ±0.001	-28.23±0.004
0.5	-28.64±0.02	-20.85±0.01	-19.99±0.03	-19.56±0.004
1.0	-22.00±0.01	-15.01±0.01	-14.50±0.01	-14.44±0.02
2.0	-16.20±0.03	-10.01±0.02	-9.99±0.01	-12.76±0.02
3.0	-15.46±0.01	-9.88±0.02	-9.86±0.02	-11.30±0.004
D-(+)-Trehalose dehydrate				
0.0	-38.38± 0.01	-30.20 ±0.01	-28..30±0.0001	-27.75 ±0.0001
0.5	-27.85±0.03	-20.08±0.003	-18.28±0.01	-17.84±0.01
1.0	-21.40±0.03	-15.09±0.01	-13.99±0.03	-14.60±0.02
2.0	-14.55±0.02	-9.47±0.07	-9.37±0.02	-10.83±0.02
3.0	-12.95±0.01	-8.87±0.06	-8.79±0.05	-10.62±0.01
D-(+)-Raffinose pentahydrate				
0.0	-39.01± 0.01	-31.57± 0.01	-29.80± 0.02	-18.90± 0.01
0.5	-26.00± 0.03	-18.58±0.03	-17.53±0.04	-6.29±0.01
1.0	-20.92± 0.02	-14.80±0.02	-14.29±0.05	-4.37±0.04
2.0	-14.90± 0.04	-9.36±0.02	-9.27±0.02	-2.17±0.01
3.0	-12.30±0.01	-8.12±0.02	-8.09±0.02	-1.01±0.004
(+)-methyl α-D-glucopyranoside				
0.0	-24.87 ±0.01	-13.88± 0.01	-12.86± 0.001	-11.91 ±0.01
0.5	-17.87± 0.01	-7.40±0.01	-6.87±0.01	-6.49±0.02
1.0	-16.14±0.05	-5.95±0.01	-5.73±0.02	-5.50±0.02
2.0	-12.48± 0.02	-2.69±0.02	-2.45±0.003	-2.34±0.01
3.0	-10.91± 0.02	-1.25±0.01	-1.23±0.02	-1.12±0.02
Methyl α-D(+)-xylopyranoside				
0.0	-19.65± 0.01	-9.98 ±0.01	-8.89± 0.001	-7.99± 0.03
0.5	-18.32± 0.02	-8.09±0.02	-7.05±0.01	-5.70±0.01
1.0	-12.36± 0.03	-3.53±0.03	-3.48±0.02	-3.38±0.04
2.0	-10.09± 0.06	-1.80±0.03	-1.79±0.02	-1.66±0.01
3.0	-9.32± 0.05	-1.07±0.03	- 0.90±0.03	-0.84±0.03
Methyl β-D(+)-xylopyranoside				
0.0	-17.28 ±0.001	-10.44± 0.02	-8.13 ±0.01	-7.00± 0.01
0.5	-16.01± 0.02	-8.71±0.03	-5.96±0.0001	-4.09±0.0004
1.0	-10.38± 0.05	-4.63±0.06	-3.16±0.01	-2.77±0.03
2.0	-8.36± 0.05	-2.67±0.04	-1.14±0.02	-1.10±0.01
3.0	-7.56± 0.03	-2.17±0.03	-0.59±0.001	-0.54±0.002

The $K^0_{s,2}$ values can provide information about the solute-solvent interactions. The $K^0_{s,2}$ values of the saccharides can be expressed by the model reported by Millero et al [14].

$$K^0_{s,2} = K^0_{s,2}(int) + K^0_{s,2}(elect) \qquad (4)$$

where $K^0_{s,2}$ (int) is the intrinsic partial molar adiabatic compressibility and $K^0_{s,2}$ (elect) is the electrostriction partial molar adiabatic compressibilty of the saccharides. Millero et al.[14] further made an approximation that $K^0_{s,2}$ (int) ≈ 0, since one would expect $K^0_{s,2}$ (int) to be very small. The $K^0_{s,2}$ may be thought to represent $K^0_{s,2}$ (elect). The $K^0_{s,2}$ values of saccharides in water are all negative, which may be due to the hydration of saccharides, as the hydrated water molecules are already compressed and thus less compressible than that present in the bulk. The $K^0_{s,2}$ values increase from mono- to di- to trisaccharides, which may be considered to show a decreasing order of hydration for the studied saccharides.

The partial molar adiabatic compressibilities of transfer, $\Delta_t K^0_{s,2}$ at infinite dilution for the studied saccharides and

derivatives in aqueous cosolutes are ploted (only representative plots given). Plots of $\Delta_t K^0_{s,2}$ versus m_B, molality of $MgCl_2$ (Figs.1a-e) show that in monosaccharides, generally there is sharp increase in $\Delta_t K^0_{s,2}$ values at all the temperatures and the $\Delta_t K^0_{s,2}$ values decrease with temperature. In hexoses, sharp increase in $\Delta_t K^0_{s,2}$ (Figs.1c-e) values between m_B=(2.0 to 3.0) mol.kg^{-1}. It may also be noted that decrease in $\Delta_t K^0_{s,2}$ values in general is more at higher concentrations of $MgCl_2$ with temperature. The $\Delta_t K^0_{s,2}$ values in case of monosacchrides increases as: XYL<ARA < RIB < MAN< FRU< GLU< GAL. Among the disaccharides, D(+)-cellobiose and D(+)-melibiose show almost sharp increase (Figs.1f,g) in $\Delta_t K^0_{s,2}$ values at higher concentration of $MgCl_2$. In the remaining disaccharides, increase in $\Delta_t K^0_{s,2}$ values is sharp upto 0.5 mol.kg^{-1}, at all temperatures and the values increase linearly afterwards, except in cases D(+)-maltose monohydrate, D-(+)-lactose monohydrate, D(+)-trehalose dihydrate (Fig.1h, only representative plot), where the values tend to level off with the increase in temperature and concentration m_B=(2.0 to 3.0) mol.kg^{-1}. D(+)-Raffinose pentahydrate (trisaccharide) shows more or less similar behaviour to disaccharides. The $\Delta_t K^0_{s,2}$ values increase in the following order for di- and tri- saccharides: MEL< CEL < SUC < LAC < MAL < TRE< RAF. The methyl-α-D-xylo- and methyl-β-D-xylopyranosides show continuous increase in $\Delta_t K^0_{s,2}$ values (Figs.1i,j) at all temperatures. In the case of α-methyl-D(+)-glucoside, there is sharp increase in $\Delta_t K^0_{s,2}$ values (Fig.1k) m_B=(2.0 to 3.0)mol.kg^{-1}. For the methylglycosides, the $\Delta_t K^0_{s,2}$ values are found to decrease in the following order: α-Me-GLU > Me-α-XYL ≥ Me-β-XYL. It may be noted that the $\Delta_t K^0_{s,2}$ values are higher in the cases of D(+)-xylose and D(+)-glucose than their respective derivatives i.e. methyl-α-D-xylo- and methyl-β-D-xylopyranosides and α-methyl-D(+)-glucoside.
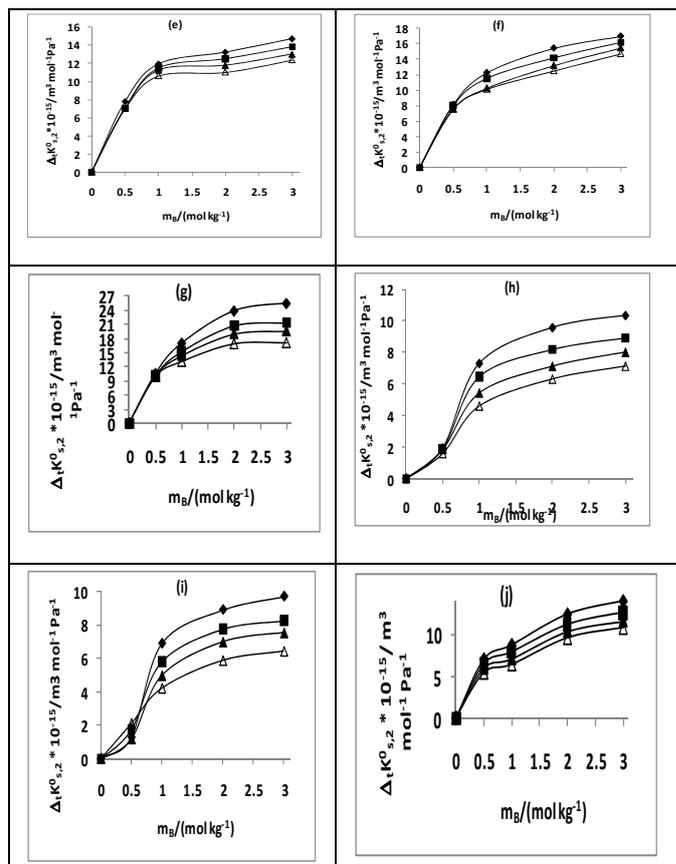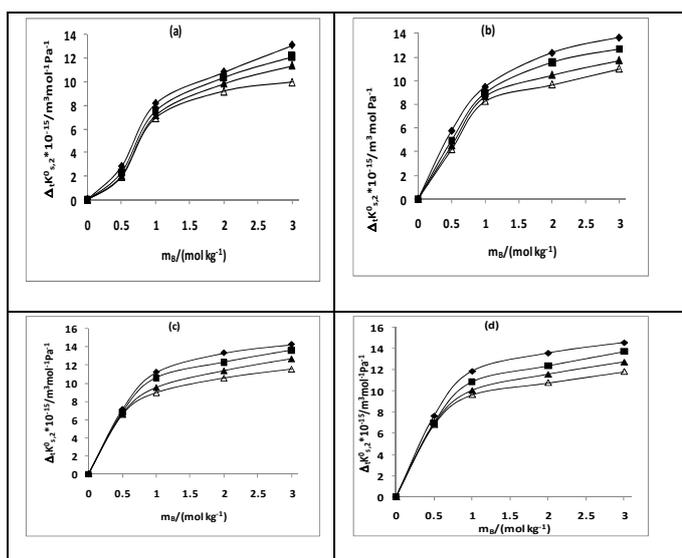

Fig. 1. plots of partial specific compressibility ΔKs,20 of MgCl2 of (a) D(−)-xylose, (b) D(−)-arabinose, (c) D-(-)- fructose (d) D-(+)-glucose (e) D-(+)- galactose, (f) D-(+)-cellobiose (g) D-(+)-trehalose dihydrate, (h) methyl α-D-xylopyranoside, (i) methyl β-D- xylopyranoside, (j) (+)-methyl α-D-glucopyranoside,at 288.15K (♦),298.15K (■), 308.15K (▲), 318.15K (Δ).

The $\Delta_t K^0_{s,2}$ values of various saccharides and methylglycosides are positive and increase with the increase in complexity of the saccharides. This suggests that an overall structural increase occurs in the solution. Similar pattern of behaviour for volumetric properties for mono-, di-, and tri- saccharides in the aqueous solutions of $MgCl_2$ has also been reported [23]. It was suggested that the hydrophilic-ionic interactions predominate over the hydrophobic-ionic interactions. An increase in the $\Delta_t K^0_{s,2}$ values from aldopentoses to hexoses, may be due to the additional –CHOH group. The lower value for D(−)-fructose than the remaining aldohexoses m ay be due to the different nature of the >C=O and –CHO groups and steric strain due to the presence of 5- membered ring in D(-) -fructose. Lower values of $\Delta_t K^0_{s,2}$ for methylglycosides; α-methyl-D(+)-glucoside / methyl-α-D-xylopyranoside/methyl-β-D-xylopyranoside than their corresponding saccharides; D(+)- glucose and D(+)-xylose may be attributed to the presence of additional –OCH$_3$ group in methylglycosides manifesting weaker hydration

compared to saccharides. Higher $\Delta_t K^0_{s,2}$ values for methyl-α-D-xylopyranoside than methyl-β-D-xylopyranoside (although difference is very small) at all concentrations (of MgCl$_2$) and temperatures reflect a change of orientation of the -OH /-OCH$_3$ group from α to β indicating weaker hydration in methyl-β-xylopyranoside than methyl-α-xylopyranoside.

The $\Delta_t K^0_{s,2}$ values are positive, and generally there is an increase in $\Delta_t K^0_{s,2}$ values with concentration of a cosolute at all the temperatures studied. Furthermore, the $\Delta_t K^0_{s,2}$ values decrease with temperature. The significant positive $\Delta_t K^0_{s,2}$ values obtained presently for the systems studied suggest that the hydrophilic-ionic interactions predominate over the hydrophobic-ionic interactions and the increase in $\Delta_t K^0_{s,2}$ values with concentration of cosolute indicates the strengthening of the hydrophilic-ionic interactions over the entire range of concentration.

The hydration numbers, n_H of saccharides were calculated using the method reported by Millero et al.[14]

$$n_H = -\frac{K^0_{s,2}\ (elect)}{K^0_s\ V^0_1} \tag{5}$$

where K^0_s and V^0_1 are compressibility and the molar volume of bulk water or bulk solvent, respectively; $K^0_{s,2}$ (elect) is the electrostriction partial molar compressibility, which is taken approximately equal to $K^0_{s,2}$ as $K^0_{s,2}$ (int) ≈ 0.

$$K^0_{s,2}(elect)=K^0_{s,2}(saccharide) \tag{6}$$

The magnitudes of n_H values are less in aqueous solutions of cosolutes as compared to those in water and decrease with the increase in concentration of cosolute. This shows that the cosolutes have dehydration effects on the saccharides. Kozak et al. proposed a formalism based on McMillan-Mayer theory of solutions, which is further discussed by Friedman and Krishnan and

Franks et al. in order to include the solute-cosolute interactions in the salvation spheres. According to this treatement, at infinite dilution, $_t K^0_{s,2}$ can be expressed as:

$$\Delta_t K^0_{s,2}=2K_{AB}m_B+3K_{ABB}m^2_B+\ldots\ldots\ldots \tag{7}$$

where A and B stands for saccharides and aqueous co-solute solutions, respectively. The pair, K_{AB} interaction coefficients are positive and triplet, K_{ABB} interaction coefficients are negative and their magnitudes increase with complexity of saccharides (table 2).

TABLE 2. PAIR,KAB, AND TRIPLET,KABB,INTERACTION COEFFICIENTS FOR VARIOUS SACCHARIDES IN AQUEOUS SOLUTIONS OF MGCL2 FROM EQUATION (7) OVER THE TEMPERATURE RANGE (288.15 TO 318.15)K

Saccharide		$K_{AB}/(m^3\ mol^{-2}\ Pa^{-1}kg)$	$K_{ABB}/(m^3\ mol^{-3}\ Pa^{-1}kg^2)$
		T=288.15 K	
D-(+)-xylose		4.1750±0.590	-0.45±0.150
D-(−)-Arabinose		5.59±0.590	-2.2527±0.130
D-(−)-ribose		6.444±0.746	-0.9357±0.190
D-(+)-mannose		6.5228±0.781	-0.9459±0.199
D-(−)-fructose		6.632±0.819	-0.967±0.208
D-(+)-galactose		6.9064±0.114	-1.02±0.283
D-(+)-glucose		6.9884±0.976	-1.039±0.248
D-(+)-melibiose		7.1136±0.851	-1.0367±0.216
D-(+)-cellobiose		7.3369± 0.882	-1.0244±0.224
D-(+)-maltose monohydrate		9.5924±.637	-1.2138±0.162
Sucrose		7.7214±0.814	-1.0731±0.207
D-(+)-lactose monohydrate		9.8971±0.823	-1.2829±0.209
D-(+)-trehalose dihydrate		10.3728±0.629	-1.3788±0.160
D-(+)-raffinose pentahydrate		11.1458±1.981	-1.5198±0.357
(+)-Methyl glucopyranoside	α-D-	5.566± 0.835	-0.736±0.212
methyl xylopyranoside	α-D-	3.1473±1.641	-0.3031±0.417
Methyl xylopyranoside	β-D-	2.9031±1.623	-0.27196±0.413
		T= 298.15 K	
D-(+)-xylose		3.8972±0.594	0.4173±0.151
D-(−)-Arabinose		5.0298±0.426	-0.6565±0.108
D-(−)-ribose		5.9623±0.663	-0.8693±0.168
D-(+)-mannose		6.0166±0.728	-0.8631±0.185
D-(−)-fructose		6.1798±0.882	-0.8925±0.224
D-(+)-galactose		6.6094±0.998	-0.9941±0.254
D-(+)-glucose		6.3216±0.945	-0.9216±0.240
D-(+)-melibiose		6.6451±0.683	-0.9619±0.174
D-(+)-cellobiose		6.8405±1.013	-0.9467±0.257
D-(+)-maltose monohydrate		9.0381±0.648	-1.2133±0.165
Sucrose		7.1751±0.931	-0.9889±0.237
D-(+)-lactose monohydrate		4.4087±0.787	-1.2967±0.200
D-(+)-trehalose dihydrate		9.3481±0.808	-1.2468±0.205
D-(+)-raffinose pentahydrate		12.2140±1.502	-1.5438±0.382
(+)-Methyl glucopyranoside	α-D-	5.0734±0.804	-0.675±0.204
methyl xylopyranoside	α-D-	2.501±1.662	-0.2345±0.422
Methyl xylopyranoside	β-D-	2.3599±1.594	-0. 2026±0.405
		T=308.15K	
D-(+)-xylose		3.834± 0.618	-0.3969±0.157
D-(−)-Arabinose		4.8512± 0.533	-0.6574±0.136
D-(−)-ribose		5.6109±0.689	-0.8202±0.175
D-(+)-mannose		5.8250±0.734	0.8583±0.187
D-(−)-fructose		5.6749±0.861	-0.8129±0.219
D-(+)-galactose		5.4084±1.099	-0.97±0.280
D-(+)-glucose		5.9395±0.939	-0.8707±0.239
D-(+)-melibiose		6.1171±0.796	-0.88±0.200
D-(+)-cellobiose		6.2051±1.026	-0.8299±0.2607
D-(+)-maltose monohydrate		8.404±0.742	-1.1913±0.1885
Sucrose		6.7266±0.887	-0.9239±0.225
D-(+)-lactose monohydrate		8.6519±0.908	-1.2362±0.231
D-(+)-trehalose dihydrate		8.9895±0.933	-1.2963±0.237
D-(+)-raffinose pentahydrate		9.8231±1.615	-1.4629±0.410
(+)-Methyl glucopyranoside	α-D-	4.6486±0.739	-0.615±0.188
methyl xylopyranoside	α-D-	0.9999 ± 1.521	-0.1350±0.387
Methyl xylopyranoside	β-D-	1.887±1.747	0.1226±0.406
		T=318.15K	
D-(+)-xylose		3.5079 ±0.620	0.38±0.160
D-(−)-Arabinose		4.54±0.570	-0.62±0.150
D-(−)-ribose		5.45±0.740	-0.81±0.190
D-(+)-mannose		5.65±0.760	-0.85±0.190
D-(−)-fructose		5.42±0.880	-0.80±0.220

D-(+)-galactose		6.07±1.130	-0.92±0.290
D-(+)-glucose		5.72±0.980	-0.86±0.250
D-(+)-melibiose		5.72±0.810	-0.82±0.200
D-(+)-cellobiose		5.21±1.500	-0.47±0.380
D-(+)-maltose monohydrate		7.57±0.944	-1.095±0.240
Sucrose		6.3143±0.887	-0.8640±0.225
D-(+)-lactose monohydrate		7.8204±1.106	-1.1398±0.281
D-(+)-trehalose dihydrate		8.4136±1.094	-1.2590±0.278
D-(+)-raffinose pentahydrate		9.2805±2.000	-1.44±0.510
(+)-Methyl glucopyranoside	α-D-	4.117±0.716	-0.5435±0.182
Methyl xylopyranoside	α-D-	1.5132 ±1.510	-0.07926±0.384
Methyl xylopyranoside	β-D-	1.3404±1.699	-0.04516±0.432

In the present work, the method reported by Surdo et al. has been used for the estimation of hydration numbers. However, instead of partial molar adiabatic compressibilities ($K_{s,2}^0$) used in their method, the hydration numbers have been estimated using partial molar isothermal compressibilities ($K_{T,2}^0$) of saccharides as follows.

$$n_H = K_{T,2}^0(elect)/V^0.K_T^0)$$
(8)

Where, $K_{T,2}^0(elect)/V^0.K_T^0)$

Where, $K_{s,2}^0$ and V^0 are the isothermal compressibility and molar volume of pure water at 298.15K.

The following general observations have been made from the comparison of comparison results for various saccharides and methylglycosides with the corresponding volumetric results in aqueous MgCl$_2$ solutions [23] at (288.15 to 318.15) K:

(i) $\Delta K_{s,2}^0$ values of various saccharides and methylglycosides increase systematically with their complexity from mono-, to di-, to tri-saccharides and with the concentrations of MgCl$_2$.

(ii) Both compressibility and volumetric studies support earlier conclusion that solute-co-solute interactions are stronger in the case of D(+)-maltose monohydrate and weaker in the case of D(+)-cellobiose.

REFERENCES

[1] 1. S. A. Galema, M. J. Blandamer, J. B. F. N. Engberts, J. Am. Chem. Soc. 112, 1990, 9665.

[2] S. A. Galema, M. J. Blandamer, J. B. F. N. Engberts, J. Org. Chem. 57, 1992, 1995.

[3] S. A. Galema, H. Hoiland, J. Phys. Chem. 95, 1991, 5321.

[4] A. Kobata, Acc. Chem. Res. 26, 1993, 319.

[5] I. Ivarorka, J. P. Carver, J. Phys. Chem. 99, 1995, 6234.

[6] R. J. Woods, R. A. Dwek, C. J. Edge, B. F. Reid, J. Phys. Chem. 99, 1995, 3832.

[7] G. G. Birch, J. Grigor, W. Derbyshire, J. Sol. Chem. 18, 1989, 795.

[8] H. B. Bull, K. Breese, Biopolymers 17, 1978, 212.

[9] J. F. Back, D. Oakenfull, M. B. Smith, Biochem. 18, 1979, 5191.

[10] T. S. Lakshmi, P. K. Nandi, J. Sol. Chem. 7, 1978, 283.

[11] R. D. Lins, C. S. Pereira, P. H. Hunenberger, Protein; Structure, Function and Bioinformatics 55, 2004, 177.

[12] Q. Liu, R. K. Schmidt, B. Teo, P. A. Karplus, J. W. Brady, J. Am. Chem. Soc. 119, 1997, 7851.

[13] P. K. Banipal, A. K. Chahal, T. S. Banipal, J. Chem. Thermodyn. 41, 2009, 452- 483.

[14] F. J. Millero, A. L. Surdo, C. Shin, J. Phys. Chem. 82, 1978, 784-792.

[15] K. Zhuo, Q. Liu, Y. Wang, Q. Ren, J. Wang, J. Chem. Eng. Data 51, 2006, 919-927.

[16] R. N. Goldberg, Y. B. Tewari, J. Phys. Chem. Ref. Data 18, 1989, 809-880.

[17] B. R. Brown, S. P. Ziemer, T. L. Niederhauser, E. M. Wooley, J. Chem. Thermodyn. 37, 2005, 843-853.

[18] P. K. Banipal, V. Singh, T. S. Banipal, J. Chem. Thermodyn. 42, 2010, 90-103.

[19] P. K. Banipal, V. Singh, G. Kaur, M. Kaur, T. S. Banipal, J. Chem. Eng.Data 53,2008, 1713-1724.

[20] P. K. Banipal, H. S. Dhanjun, S. Sharma, H. Hundal, T. S. Banipal, J. Phys.Chem. 222, 2008, 177-204.

[21] P. K. Banipal, T. S. Banipal, J. C. Ahluwalia, B. S. Lark, J. Chem. Thermodyn. 34, 2002, 1825-1846.

[22] K. Zhuo, Y.Chen, W. Wang, J. Wang, J. Chem. Eng. Data 53, 2008, 2022–2028.

[23] P. K. Banipal, A. K. Chahal Nee Hundal, T. S. Banipal, Carbohydr. Res. 345, 2010, 2262-2271.