Supporting Information

Densities and Speeds of Sound of D(+)-Glucose, D(-)-Fructose, D(+)-Xylose and D(-)-Ribose in Aqueous Tripotassium Citrate Solutions at Different Temperatures

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Partial molar volumes and partial molar isentropic compression of transfer

The standard partial molar volume of transfer, ΔV_{ϕ}^{0} and partial molar isentropic compression of transfer $\Delta K_{\phi,S}^{0}$ at infinite dilution for all the saccharides from water to aqueous solution of TPC have been calculated as

$$\Delta V_{\phi}^{0} = V_{\phi}^{0} \text{ (in aqueous TPC solutions)} - V_{\phi}^{0} \text{ (in water)} \qquad \text{(E1)}$$

$$\Delta K_{\phi,S}^{0} = K_{\phi,S}^{0} \text{ (in aqueous TPC solutions)} - K_{\phi,S}^{0} \text{ (in water)} \qquad \text{(E2)}$$

These values of ΔV_{ϕ}^{0} and $\Delta K_{\phi,S}^{0}$ have been reported in Table S1.

Apparent Specific Volumes

Apparent specific volumes of two monosaccharides in aqueous solutions of tripotassium citrate have been calculated at T = (288.15, 298.15, 308.15, and 318.15) K by using following equation:

$$\nu_{\phi} = V_{\phi}/\mathrm{M} \qquad \text{(E3)}$$

Temperature dependence of partial molar volume

Further, the variation of apparent molar volumes at infinite dilution V_ϕ^0 with the temperature can be expressed by the general polynomial equation as follows

$$V_\phi^0 = a + b\,(T - T_{\mathrm{ref}}) + c\,(T - T_{\mathrm{ref}})^2 \qquad \text{(E4)}$$

Where T is temperature in Kelvin. T_{ref} = 298.15 K. a, b, and c are empirical constants. The values of these constants for saccharides in aqueous trisodium citrate solutions are reported in Table S2. The values of V_ϕ^0 were calculated with these parameters and deviations obtained from experimental and calculated values are also reported in Table S2. The deviations are calculated as follows

$$\sigma = (1/n)\,\Sigma\,[\mathrm{abs}((Y_{\mathrm{exptl.}} - Y_{\mathrm{calc.}}) / Y_{\mathrm{exptl.}})] \qquad \text{(E5)}$$

where $Y = V_\phi^0$ (apparent molar volume at infinite dilution). The values reported in Table S2 for ARD are very small which predicts the polynomial equation very well.

The limiting apparent molar expansibilities are calculated as follows

$$\phi_E^0 = (\partial V_\phi^0 / \partial \mathrm{T})_p = \mathrm{b} + 2\,\mathrm{c}\,(T - T_{\mathrm{ref}}) \qquad \text{(E6)}$$

Hepler[50] developed the general thermodynamic expression to determine capacity of solute as structure maker or structure breaker in mixed solvent system using general thermodynamic expression

$$(\partial \phi_E^0 / \partial \mathrm{T})_p = \left(\partial^2 V_\phi^0 / \partial T^2\right)_p = 2\,\mathrm{c} \qquad \text{(E7)}$$

The values of limiting apparent molar expansibilities ϕ_E^0 and $(\partial \phi_E^0 / \partial \mathrm{T})_p$ are reported in Table S3.

Pair and triplet interaction coefficients

Interaction coefficients have been calculated based upon the McMillan-Mayer theory of solutions[52,53] which permits the separation of effects due to interaction between the pairs of solute molecules and those due to its interaction between more than two solute molecules. Same approach has further been discussed by Friedmann & Krishnan[54] and Franks *et al.*[55] in order to include solute-cosolute interactions in the solvation spheres. So, thermodynamic transfer function at infinite dilution *i.e.* partial molar volume of transfer and partial molar isentropic compression of transfer can be expressed as follows:

$$\Delta V_{\phi}^{0} \text{ (water to aqueous TPC solution)} = 2\, V_{AB} m_{B} + 3\, V_{ABB}\, m_{B}^{2} + \ldots\ldots \quad \text{(E8)}$$

$$\Delta K_{\phi,S}^{0} \text{ (water to aqueous TPC solution)} = 2\, K_{AB} \mathrm{m}_{B} + 3\, K_{ABB}\, m_{B}^{2} + \ldots\ldots.. \quad \text{(E9)}$$

where A denotes saccharide, B denotes TPC and m_B is the molality of TPC. The corresponding parameters V_{AB}, V_{ABB} for volume and K_{AB}, K_{ABB} for isentropic compression denotes pair and triplet interaction coefficients for studied saccharides respectively. These constants were calculated by fitting the ΔV_{ϕ}^{0} and $\Delta K_{\phi,S}^{0}$ values to the above equation. The values are reported in Table S4.

Table S1. Partial Molar Volume of Transfer, ΔV_{ϕ}^{0} and Partial Molar Isentropic Compression of Transfer, $\Delta K_{\phi,S}^{0}$ of Monosaccharides in Aqueous Tripotassium Citrate Solutions over the Temperature Range (288.15 to 318.15) K

$^{a}m_{B}$ mol·kg^{-1}	$\Delta V_{\phi}^{0} \times 10^{6}$ m^{3}·mol^{-1}				$\Delta K_{\phi,S}^{0} \times 10^{6}$ m^{3}·mol^{-1}·GPa^{-1}			
	T = 288.15 K	T = 298.15 K	T = 308.15 K	T = 318.15 K	T = 288.15 K	T = 298.15 K	T = 308.15 K	T = 318.15 K
D(+)-Glucose								
0.2	2.58	2.70	2.38	2.06	10.64	9.00	8.09	7.69
0.4	4.50	4.28	3.91	3.73	17.15	14.38	12.41	12.22
0.6	5.09	4.98	4.42	4.17	26.26	22.96	20.60	19.29
D(-)-Fructose								
0.2	0.76	1.45	1.61	2.18	9.67	7.46	7.34	7.17
0.4	1.57	1.99	1.92	2.16	15.50	12.48	10.99	10.72
0.6	2.36	2.49	2.38	2.68	25.77	22.14	20.09	18.95
D(+)-Xylose								
0.2	0.86	0.52	0.78	0.87	8.41	6.02	5.85	5.37
0.4	1.69	1.06	1.28	1.22	11.66	8.68	7.94	7.26
0.6	1.82	1.32	1.71	1.93	17.71	14.88	12.96	11.80
D(-)-Ribose								

0.2	0.95	1.40	1.11	2.25	9.30	7.23	6.64	7.74
0.4	1.69	1.73	1.66	2.68	12.23	9.53	8.18	8.09
0.6	2.63	2.81	2.71	3.98	19.59	16.69	14.50	13.89

[a]m_B is the molality of aqueous tripotassium citrate solutions

Table S2. Values of *a*, *b* and *c* Parameters of Monosaccharides in Aqueous Tripotassium Citrate Solutions

$^{a}m_B$ mol·kg^{-1}	$a \times 10^6$ m^3·mol^{-1}	$b \times 10^6$ m^3 mol^{-1} K^{-1}	$c \times 10^6$ m^3 mol^{-1} K^{-2}	R^2	ARD
D(+)-Glucose					
0.0	111.83	0.09042	0.00043	0.9999	0.00033
0.2	114.46	0.08238	-0.00067	0.9999	0.00003
0.4	116.06	0.06299	0.00050	0.9999	0.00268
0.6	116.70	0.06070	0.00008	0.9999	0.00048
D(-)-Fructose					
0.0	111.27	0.07988	0.00005	0.9999	0.00028
0.2	112.57	0.12682	-0.00021	0.9999	0.00057
0.4	113.13	0.10085	-0.00037	0.9999	0.00043
0.6	113.66	0.08413	0.00048	0.9999	0.00031
D(+)-Xylose					
0.0	95.54	0.11258	-0.00248	0.9999	0.00121
0.2	96.17	0.10449	-0.00138	0.9999	0.00001
0.4	96.76	0.08594	-0.00102	0.9999	0.00041

0.6	97.02	0.10176	-0.00067	0.9999	0.00030
D(-)-Ribose					
0.0	96.03	0.09882	-0.00219	0.9999	0.00096
0.2	97.10	0.11758	-0.00045	0.9999	0.00291
0.4	97.57	0.10346	0.00028	0.9999	0.00203
0.6	98.59	0.11119	0.00055	0.9999	0.00237

Table S3. Limiting Apparent Molar Expansibilities (ϕ_E^0) and its Derivative $(\partial \phi_E^0 / \partial T)_p$ of Monosaccharides in Aqueous Tripotassium Citrate Solutions over the Temperature Range (288.15 to 318.15) K.

$^a m_B$ mol·kg^{-1}	$\phi_E^0 \times 10^6$ (m^3·mol^{-1}·K^{-1})				$(\partial \phi_E^0 / \partial T)_p$ (m^3·mol^{-1}·K^{-2})
	T = 288.15 K	T = 298.15 K	T = 308.15 K	T = 318.15 K	
D(+)-Glucose					
0.0	0.082	0.090	0.099	0.107	0.00080
0.2	0.096	0.082	0.069	0.056	-0.00134
0.4	0.053	0.063	0.073	0.083	0.00101
0.6	0.059	0.065	0.066	0.068	0.00015
D(-)-Fructose					
0.0	0.079	0.080	0.081	0.082	0.00010
0.2	0.131	0.127	0.123	0.118	-0.00043
0.4	0.108	0.101	0.093	0.086	-0.00075
0.6	0.074	0.084	0.094	0.103	0.00097
D(+)-Xylose					
0.0	0.150	0.110	0.070	0.03	-0.0040
0.2	0.132	0.104	0.077	0.049	-0.00275
0.4	0.106	0.086	0.066	0.045	-0.00204
0.6	0.115	0.102	0.088	0.075	-0.00134
D(-)-Ribose					
0.0	0.14	0.100	0.060	0.020	-0.0040

0.2	0.127	0.122	0.113	0.104	-0.0009
0.4	0.098	0.103	0.109	0.115	0.00056
0.6	0.100	0.115	0.126	0.137	0.00109

Table S4. Pair Interaction (V_{AB}, K_{AB}) and Triplet Interaction (V_{ABB}, K_{ABB}) Coefficients for Monosaccharides in Aqueous Tripotassium Citrate Solutions over the Temperature Range (288.15 to 318.15) K

T (K)	V_{AB}	V_{ABB}	K_{AB}	K_{ABB}
D(+)-Glucose				
288.15	7.93±0.43	-4.07±0.54	23.13±4.39	-3.94±5.53
298.15	7.91±0.15	-4.18±0.19	20.28±4.44	-1.61±5.60
308.15	7.18±0.13	-3.87±0.16	17.40±4.96	-0.63±6.25
318.15	6.45±0.55	-3.27±0.70	17.54±3.70	-1.91±4.67
D(-)-Fructose				
288.15	1.91±0.63	0.063±0.08	20.80±5.38	0.35±6.78
298.15	3.89±0.56	-2.06±0.71	14.70±4.61	3.82±5.80
308.15	4.22±0.94	-2.55±1.18	13.93±5.95	2.68±7.40
318.15	5.49±1.80	-3.76±2.26	14.26±5.41	1.30±6.82
D(+)-Xylose				
288.15	2.85±0.44	-1.45±0.56	19.63±5.19	-5.79±6.54
298.15	1.56±0.18	-0.49±0.23	12.43±4.50	-0.37±5.67
308.15	2.09±0.13	-0.75±0.17	12.73±4.35	-2.46±5.46
318.15	1.95±0.58	-0.42±0.73	11.73±4.00	-2.41±5.04
D(-)-Ribose				

288.15	2.23±0.28	-0.07±0.35	20.56±7.04	-5.24±8.87
298.15	3.05±1.19	-0.87±1.50	14.58±6.37	-1.22±8.03
308.15	2.42±0.69	-0.23±0.87	13.21±6.44	-1.73±8.11
318.15	5.25±1.75	-2.28±2.20	15.93±8.36	-5.46±10.54