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Volumetric, ultrasonic and viscometric studies of solute–solute and solute–solvent interactions of *l*-threonine in aqueous-sucrose solutions at different temperatures

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ABSTRACT

Densities, ρ of solutions of *l*-threonine in aqueous-sucrose solvents 5%, 10%, 15%, and 20% of sucrose, w/w in water at $T = (293.15, 298.15, 303.15, 308.15, 313.15,$ and $318.15)$ K; and ultrasonic speeds, u and viscosities, η of these solutions at 298.15, 303.15, 308.15, 313.15, and 318.15 K were measured at atmospheric pressure. From these experimental results, the apparent molar volume, V_ϕ, limiting apparent molar volume, V_ϕ° and the slope, S_v, apparent molar compressibility, $K_{s,\phi}$, limiting apparent molar compressibility, $K_{s,\phi}^\circ$ and the slope, S_k, transfer volume, $V_{\phi,tr}^\circ$, transfer compressibility, $K_{s,\phi,tr}^\circ$, limiting apparent molar expansivity, E_ϕ°, Hepler's constant, $(\partial^2 V_\phi^\circ/\mathrm{d}T^2)$, Falkenhagen coefficient, A, Jones–Dole coefficient, B and hydration number, n_H have been calculated. The results have been interpreted in terms of solute–solvent and solute–solute interactions in these systems. The Gibbs energies of activation of viscous flow per mole of solvent, $\Delta\mu_1^{\circ\#}$ and per mole of solute, $\Delta\mu_2^{\circ\#}$ were also calculated and discussed in terms of transition state theory. It has been observed that there exist strong solute–solvent interactions in these systems and these interactions increase with increase in sucrose concentration in solution.

1. Introduction

The stabilization of native conformations of biological macromolecules (proteins) is related to several non-covalent interactions including hydrogen-bonding, electrostatic and hydrophobic interactions [1,2]. These interactions are affected by the surrounding solute and solvent molecules; for this reason, the physicochemical properties of proteins are strongly affected by the presence of these solutes. Because of direct solute–solvent interactions and/or alteration of the water structure, these solutes can change many properties of globular proteins, such as their hydration, solubility and the activity of enzymes [3–6]. These interactions are important in understanding the stability of proteins, and are implicated in several biochemical and physiological processes in a living cell [7–10]. In continuation to our earlier studies [11–14] on the interactions of amino acids in aqueous-carbohydrate solutions, here we report the results of our study on volumetric, acoustic and viscometric behaviour of *l*-threonine in aqueous-sucrose solutions.

It is known [8,9,15,16] that polyhydroxy compounds help in stabilizing the native globular structure of protein and reduce the extent of their denaturation by other substances. Carbohydrates located at cell surfaces, are important as receptors for the bioactive structures of enzymes, hormones, viruses, antibodies, *etc.* [17]. The protein–carbohydrate interactions are important for immunology, biosynthesis, pharmacology, medicine, and cosmetic industry [18,19]. Thus, the properties of amino acids in aqueous-carbohydrate solutions are essential for understanding the chemistry of biological systems [20,21].

In the present article, we report the densities, ρ, ultrasonic speeds, u and viscosities, η of solutions of *l*-threonine in aqueous-sucrose solvents 5%, 10%, 15%, and 20% of sucrose, w/w in water at different temperatures and atmospheric pressure. Various physicochemical parameters, *viz.*, V_ϕ, V_ϕ°, $K_{s,\phi}$, $K_{s,\phi}^\circ$, $V_{\phi,tr}^\circ$, $K_{s,\phi,tr}^\circ$, E_ϕ°, $(\partial^2 V_\phi^\circ/\mathrm{d}T^2)$, A, B, n_H, $\Delta\mu_1^{\circ\#}$ and $\Delta\mu_2^{\circ\#}$ have been calculated using the experimental data. The results have been interpreted in terms of solute–solvent and solute–solute interactions in these systems.

2. Experimental

l-Threonine (SRL India, mass fraction purity > 0.99) was used after re-crystallization from ethanol–water mixture and dried in vacuum over P_2O_5 at room temperature for 72 h (table 1). Sucrose (E. Merck, Germany, mass fraction purity > 0.998) was used as such without further purification, except drying in oven for 24 h (table 1). The aqueous-sucrose solutions 5%, 10%, 15%, and 20% of sucrose, w/w in water were prepared using triple distilled water (conductivity less than 1×10^{-6} S · cm^{-1}) and these were used as solvents to prepare *l*-threonine solutions of eight different molal concentrations (ranging from 0 to 0.2 m). The weighing was done on an

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TABLE 1
Provenance and purity of the chemical samples studied.

Chemical name	Provenance	Purification method	Final mass fraction purity	Analysis method
l-Threonine	SRL, India	Re-crystallization	>0.993	GC[a]
Sucrose	E. Merck, Germany	Used as received	>0.998	

[a] GC = gas chromatography.

electronic balance (Model: GR-202R, AND, Japan) with a precision of ±0.01 mg. The solutions were prepared with care and stored in special airtight bottles to avoid contamination and evaporation.

The densities of the sample solutions were measured by using a single-capillary pycnometer (made of Borosil glass) having a bulb capacity of ~10 mL. The capillary, with graduated marks, had a uniform bore and could be closed by a well-fitting glass cap. The marks on the capillary were calibrated by using triply distilled water. The uncertainty in density measurements was estimated to be ±0.02 kg · m^{-3}. The ultrasonic speeds in the solutions were measured using a single-crystal variable-path multi-frequency ultrasonic interferometer (Model: M-81DS, Mittal Enterprises, India) having stainless steel sample cell (with digital micrometer) operating at 3 MHz. The uncertainty in ultrasonic speed measurements was within ±0.3 m · s^{-1}. The viscosities of the solutions were measured by using Ubbelohde type suspended level viscometer. The viscometer containing the test liquid was allowed to stand for about 30 min in a thermostatic water bath so that the thermal fluctuations in viscometer were minimized. The time of flow were recorded in triplicate with a digital stopwatch with an accuracy of ±0.01 s. The accuracy of viscosity measurements was estimated to be ±1 × 10^{-6} N · s · m^{-2}. The temperature of the test solutions during the measurements was maintained to an accuracy of ±0.01 K in an electronically controlled thermostatic water bath (JULABO, Model: ME-31A, Germany).

3. Results

The experimental values of density, ρ, ultrasonic speeds, u, and viscosity, η of *l*-threonine solutions in aqueous-sucrose solvents as functions of *l*-threonine concentration and temperature are listed in tables 2–4, respectively.

The apparent molar volume, V_ϕ and apparent molar compressibility, $K_{s,\phi}$ of the solutions were calculated by using the relations

$$V_\phi = \frac{1000(\rho_o - \rho)}{m\rho\rho_o} + \frac{M}{\rho}, \quad (1)$$

TABLE 2
Densities, ρ/kg · m^{-3} of solutions of *l*-threonine in (sucrose + water) 5%, 10%, 15%, and 20% sucrose, w/w in water, solvents as functions of molality, m of *l*-threonine at different temperatures and at atmospheric pressure.[a]

m/mol · kg^{-1}	ρ/kg · m^{-3}					
	T = 293.15 K	T = 298.15 K	T = 303.15 K	T = 308.15 K	T = 313.15 K	T = 318.15 K
			l-Threonine in 5% aqueous-sucrose			
0.0000	1018.91	1017.19	1015.45	1013.72	1011.98	1010.23
0.0249	1019.85	1018.13	1016.39	1014.66	1012.93	1011.18
0.0498	1020.78	1019.06	1017.32	1015.59	1013.86	1012.11
0.0749	1021.69	1019.97	1018.23	1016.50	1014.77	1013.02
0.0999	1022.58	1020.86	1019.12	1017.39	1015.66	1013.92
0.1250	1023.46	1021.73	1019.99	1018.26	1016.53	1014.80
0.1499	1024.32	1022.59	1020.85	1019.13	1017.40	1015.66
0.1749	1025.16	1023.43	1021.69	1019.97	1018.24	1016.50
0.1999	1025.99	1024.26	1022.52	1020.79	1019.06	1017.33
			l-Threonine in 10% aqueous-sucrose			
0.0000	1039.28	1037.45	1035.61	1033.76	1031.93	1030.09
0.0249	1040.11	1038.28	1036.44	1034.59	1032.76	1030.92
0.0499	1040.93	1039.09	1037.25	1035.40	1033.57	1031.74
0.0749	1041.73	1039.90	1038.05	1036.20	1034.37	1032.54
0.0999	1042.51	1040.68	1038.83	1036.98	1035.16	1033.32
0.1250	1043.28	1041.44	1039.60	1037.75	1035.93	1034.09
0.1499	1044.04	1042.20	1040.35	1038.51	1036.68	1034.85
0.1750	1044.78	1042.94	1041.10	1039.25	1037.43	1035.59
0.1999	1045.51	1043.67	1041.82	1039.97	1038.15	1036.33
			l-Threonine in 15% aqueous-sucrose			
0.0000	1060.31	1058.49	1056.67	1054.84	1053.01	1051.20
0.0249	1061.04	1059.22	1057.40	1055.57	1053.74	1051.92
0.0499	1061.76	1059.94	1058.11	1056.28	1054.45	1052.64
0.0749	1062.47	1060.64	1058.82	1056.98	1055.15	1053.34
0.0999	1063.16	1061.33	1059.50	1057.67	1055.84	1054.03
0.1250	1063.84	1062.01	1060.18	1058.35	1056.52	1054.71
0.1499	1064.51	1062.68	1060.85	1059.02	1057.18	1055.37
0.1750	1065.16	1063.33	1061.50	1059.67	1057.84	1056.03
0.1999	1065.80	1063.97	1062.14	1060.31	1058.48	1056.67
			l-Threonine in 20% aqueous-sucrose			
0.0000	1082.73	1080.77	1078.80	1076.84	1074.88	1072.93
0.0250	1083.38	1081.41	1079.44	1077.48	1075.52	1073.56
0.0499	1084.01	1082.04	1080.07	1078.11	1076.14	1074.19
0.0750	1084.63	1082.66	1080.69	1078.72	1076.76	1074.80
0.0999	1085.24	1083.27	1081.29	1079.33	1077.36	1075.41
0.1249	1085.84	1083.87	1081.89	1079.93	1077.96	1076.00
0.1500	1086.43	1084.46	1082.48	1080.52	1078.55	1076.59
0.1749	1087.00	1085.04	1083.06	1081.10	1079.13	1077.17
0.2000	1087.56	1085.60	1083.63	1081.67	1079.70	1077.74

[a] Standard uncertainties s are $s(T)$ = ±0.01 K, $s(m)$ = ±1.0 × 10^{-4} mol · kg^{-1}, and $s(\rho)$ = ±2.0 × 10^{-2} kg · m^{-3}.