Effect of Trisodium Citrate on Volumetric and Acoustical Properties of 1, 3, 7-Trimethylxanthine in Aqueous Solutions at 30°C

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Abstract: ***In order to disclose different interactions in aqueous solutions of caffeine in1,3,7-trimethylxanthine (trisodium citrate) solutions, the density, ultrasonic velocity and refractive index of these solutions have been measured at 30°C. Apparent molar volumes and compressibilities of studied solutions were calculated form densities and ultrasonic velocities respectively. Partial molar properties were determined form concentration dependence of apparent molar properties using standard equations. The transfer volumetric and acoustical properties have been computed and all the parameters were interpreted in terms of different interactions in aqueous solutions.***

Keywords: Density, ultrasonic velocity, partial molar volume, partial molar compressibility

1. Introduction

The activity of drug in living system can be understood by hydration behavior of drug compounds in solution. Interactions in different solutions of drug are altered by presence of cosolutes, their concentration and temperature [1-4]. Thermophysical properties of solutions provide useful information about these interactions in solution [5-7]. Drug action across biological membrane can be found through drug–water interactions and their temperature dependence [5]. Caffeine [1, 3, 7-trimethylxanthine, Figure 1] is central nervous system (CNS) stimulant widely consumed as psychoactive agent [8]. It can treat the premature chronic lung disease of infancy disease and consumed as psychoactive agent [8], effective drug against some disease [9-10]. Sodium salt of citric acid are useful application in preservative, flavor, food additives, cosmetic, pharmaceutical industries and play vital role in biochemical process [11-13]. Trisodium citrate dihydrate (TSC, Figure 1) is useful in medicinal, biological and industrial processes.

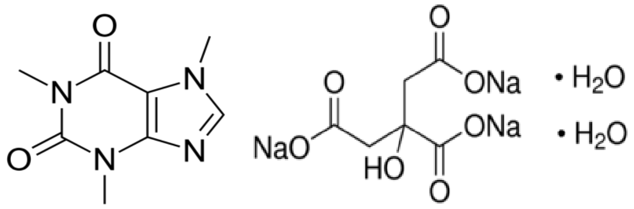


Figure 1: Structure of caffeine and trisodium citrate dihydrate

Our earlier work reports the study of pharmaceutically important drugs in solutions [14-17]. Partial molar volumes and compressibilities of aqueous-caffeine in presence of TCS solutions are lacking and it is significant to study thermodynamic properties of caffeine solutions in presence of TCS to have a detailed understanding of effect of TCS salt on hydration behavior of caffeine.

2. Experimental

Caffeine (s d Fine Limited with Minimum assay 98.5%) and trisodium citrate (Thermo Fischer Scientific with Minimum assay 99%) was used. Solutions were in double distilled water and kept in airtight bottles. Density measurements were performed using single capillary calibrated pycnometer of (10 cm^3). Single pan electronic balance (±0.0001g) was used. Ultrasonic velocity was measured using thermostatically controlled ultrasonic interferometer (Model-F05, Mittal, 2 ±0.0001 MHz). Average of 25 micrometer readings was considered. Refractive index measurements were performed on thermostatically controlled Cyber LAB-Cyber calibrated Abbe refractometer (±0.0002, 1.3000 to 1.7000).

Theoretical equations

$$V_{2,\phi} = \frac{M_2}{\rho} + \frac{1000}{m\rho\rho_0}(\rho_0 - \rho) \quad .....(1)$$

$$V_{2,\phi} = V_{2,\phi}^o + S_v c^{1/2} \quad .....(2)$$

$$\Delta_t V_{2,\phi}^o = V_{2,\phi}^o(aq.solution) - V_{2,\phi}^o(H_2O) \quad .....(3)$$

$$\kappa_s = \frac{1}{u^2\rho} \quad .....(4)$$

$$\kappa_{S,2,\phi} = \frac{1000(\kappa_s\rho_o - \kappa_o\rho)}{m\rho\rho_o} + \frac{M \times \kappa_s}{\rho} \quad .....(5)$$

$$\kappa_{S,2,\phi} = \kappa_{S,2,\phi}^0 + S_k c^{1/2} \quad .....(6)$$

$$\Delta_t \kappa_{S,2,\phi}^0 = \kappa_{S,2,\phi}^0(aq.solutions) - \kappa_{S,2,\phi}^0(H_2O) \quad .....(7)$$

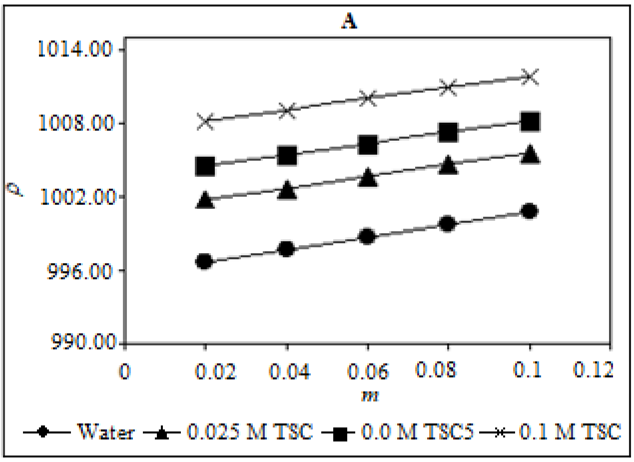
$$Z = u\rho \quad .....(8)$$

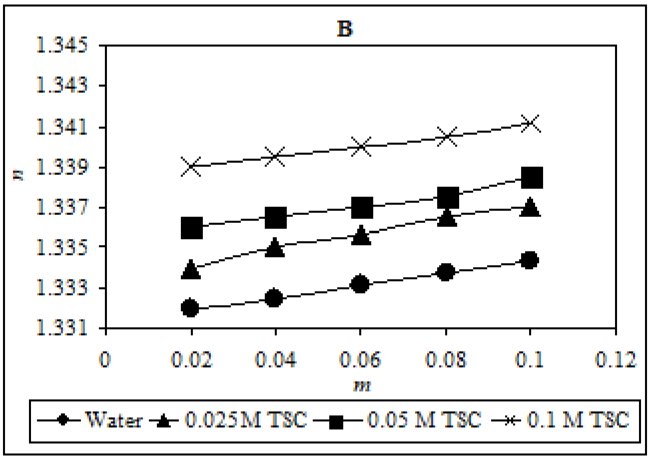
3. Results and Discussion

The experimental densities, ultrasonic velocities and refractive indices of caffeine in aqueous-TSC solutions 30°C are presented in Figure 1 A-C. These properties increase with increase in concentration of caffeine due to molecular association as a result of effective solute-solute/solvent interactions. Refractive indices trends indicate increase in compactness of solutions with concentration of solute.

Apparent molar volumes ($V_{2,\phi}$, Figure 2) and apparent molar compressibilities ($\kappa_{S,2,\phi}$, Figure 4) decrease with an increase in concentration of caffeine in each system due to strong solute-solvent interactions and these values increase with concentration of TSC due to solute-cosolute interactions and weakening of solute-solvent interactions. Isentropic compressibility (κ_S, Figure 3) decreases with increase in concentration of caffeine and TSC in each system at constant temperature. This is due to breaking of water structure around with caffeine increasing the caffeine-water and caffeine-cosolute interactions [18].

Partial molar volumes and compressibilities ($V^{o}_{2,\varphi}$ and $\kappa^{0}_{S,2,\phi}$, Table 1) and corresponding transfer volumes and compressions ($\Delta_t V^{o}_{2,\phi}$ and $\Delta_t \kappa^{0}_{S,2,\varphi}$) (Table 1) increase with concentration of TSC due to solute-cosolute interactions and weakening of solute-solvent (ion-dipole) interactions.





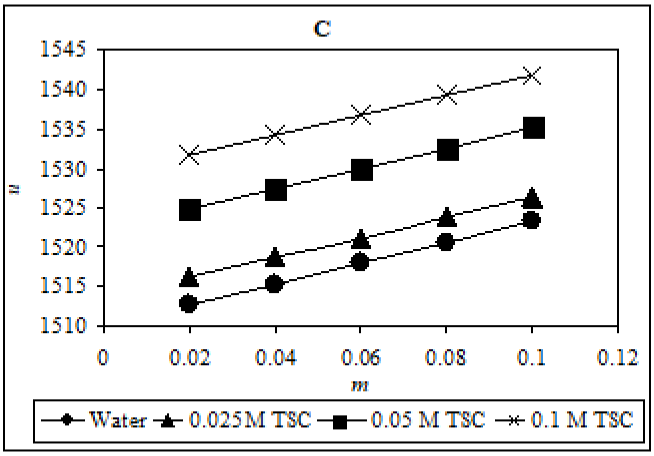


Figure 1 A-C. The experimental densities (kg·m-3), ultrasonic velocities (m·s-1) and refractive indices of caffeine + aqueous-TSC solutions 300C

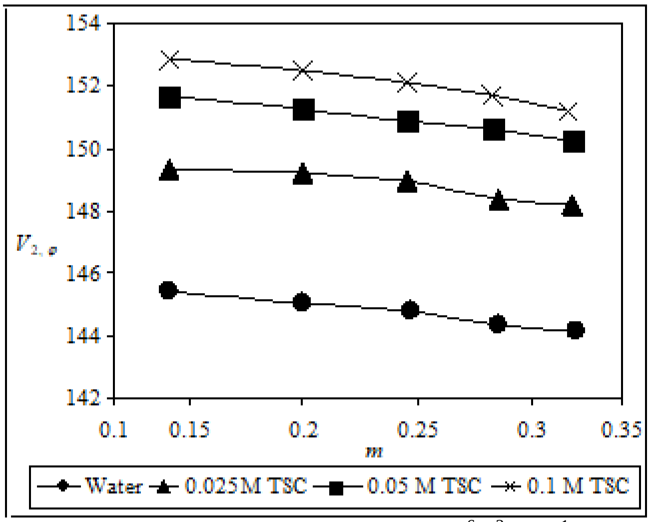


Figure 2. Apparent molar volume ($\times 10^{-6} m^3 \cdot mol^{-1}$) of solutions containing Caffeine + aqueous-TSC at 30°C

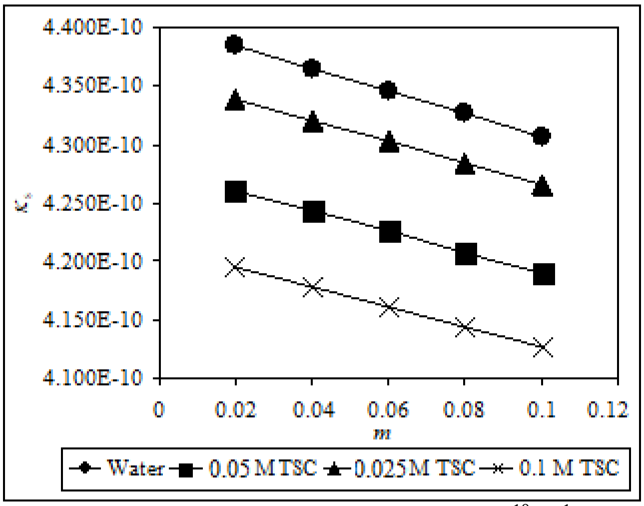


Figure 3: Isentropic compressibility ($\times 10^{-10} Pa^{-1}$) of solutions containing Caffeine + aqueous- TSC at 30°C

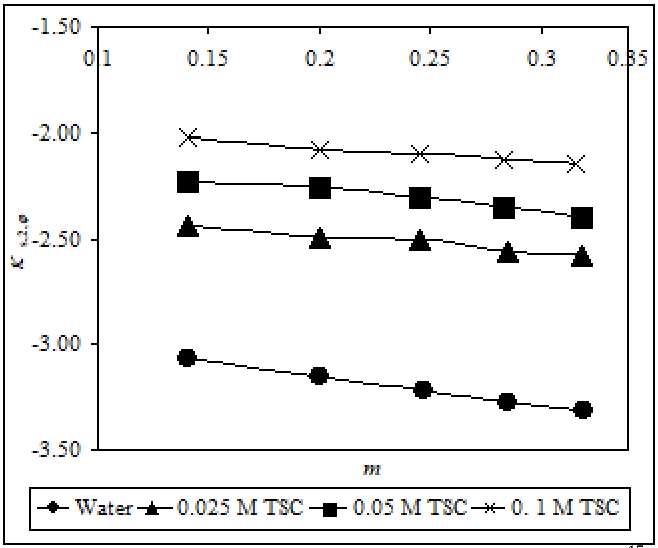


Figure 4: Apparent molar isentropic compressibility ($\times 10^{-15}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$) of caffeine + aqueous-TSC solutions 30^{0}C

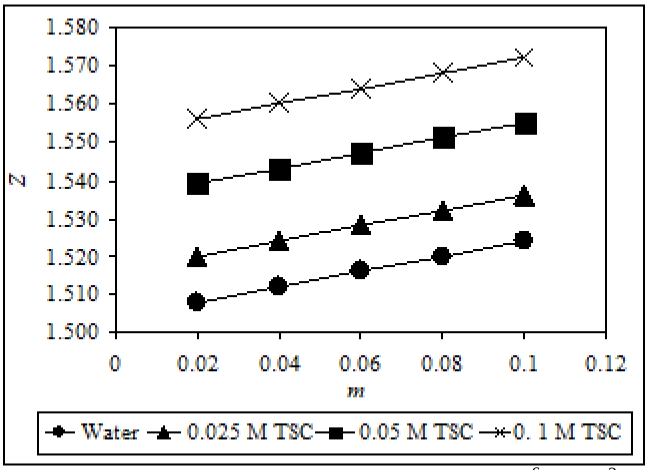


Figure 5: Specific acoustic impedance (Z, $\times 10^6$ $kg \cdot m^{-2} \cdot s^{-1}$) of caffeine + aqueous-TSC solutions 30^{0}C

Table 1: The $V^o_{2,\varphi}$, S_v and $\Delta_t V^o_{2,\varphi}$ and $\kappa^0_{S,2,\varphi}$ S_k and $\Delta_t \kappa^0_{S,2,\varphi}$ of Caffeine + aqueous-TSC at 30°C

System	$V^o_{2,\varphi}$	S_v	$\Delta_t V^o_{2,\varphi}$
Water/0.000 M aq. TSC	146.54	-7.37	0.00
0.025 M aq. TSC	150.53	-7.15	3.99
0.050M aq. TSC	152.75	-7.62	6.21
0.100 M aq. TSC	154.20	-9.08	7.66
	$\kappa^0_{S,2,\varphi}$	S_k	$\Delta_t \kappa^0_{S,2,\varphi}$
Water/0.000 M aq. TSC	-2.87	-1.41	0.00
0.025 M aq. TSC	-2.32	-0.77	-0.54
0.050M aq. TSC	-2.07	-0.98	-0.80
0.100 M aq. TSC	-1.93	-0.68	-0.94

Foot Note: $V^o_{2,\varphi}$ = $m^3 \cdot mol^{-1}$, S_v = $m^3 \cdot mol^{-3/2} \cdot kg^{1/2}$, $\kappa^0_{S,2,\varphi}$ =$\times 10^{-14}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$, S_k = $\times 10^{-14}$ $m^3 \cdot mol^{-3/2} \cdot kg^{1/2} \cdot Pa^{-1}$.

Weak solute-solute interactions are observed from S_v and S_k values (small negative) obtained from slope of the plots of $V_{2,\phi}$ vs. $\sqrt{m}$ and $\kappa_{S,2,\phi}$ vs. $\sqrt{m}$ respectively.

Specific acoustic impedance (Z, Figure 5) is product of density and ultrasonic velocity [19]. Z values increases with increase in concentration of caffeine as well as TSC which suggest significant change in the molecular interaction between caffeine and TSC salt [20-21]. The trends in Z values meant for more propagation and strong caffeine-TSC interactions.

4. Conclusion

The refractive index data shows linear dependence over the drug concentration at constant temperatures, which is well in accordance with the data obtained from volumetric and acoustical study. The observed positive values of $V^o_{2,\phi}$ and decreasing trend in S_v for caffeine drug in aqueous-TSC suggest that presence of effective solute-solvent and weak solute-solute interaction in these system. The negative values of $\kappa^0_{S,2,\phi}$ are attributed to the strong drug-solvent interactions in the solution and water molecules in the bulk solution are more compressible than water molecules surrounding the hydrophilic groups of solute. Positive values of $\Delta_t V^o_{2,\phi}$ suggest electrosrictive effect of caffeine reduces on addition of cosolute.

Conflict of interest:
The authors have no conflicts of interest regarding this investigation.

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