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Correlation Between Surface Tension On β -Cyclodextrin With Heterocyclic Compound At Various Temperatures.

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ABSTRACT

The ultrasonic velocity (U), viscosity (η) and density (ρ) of aqueous solution of β -cyclodextrin (β -CD) with tetrahydrofuran (THF) are measured at various mole fractions and various temperatures at 303.15 K-313.15 K. From the experimental data, the adiabatic compressibility (β), free volume (V_F), internal pressure (π_i), and acoustic impedance (Z) are determined. The detected results are used to study the structural transform around the ion and reaction of the solvent.

Keywords: Ultrasonic spectroscopy, Beta Cyclodextrin (β -CD), Tetra hydro furan (THF) and Surface tension.

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INTRODUCTION

Tetra hydro furan (THF) is a color less, less oily, watery heterocyclic ether. This is a versatile solvent of industrial process involving butan-1, 4-diol acid-catalytic dehydration. This is much more basic than the diethyl ether and creates strong complexes with Li, Mg and Boranes.

THF is a popular solvent for component compounds such as hydroboration reactions and organo lithium and Grignard reagent. The current trial is in the included β -cyclodextrin (β -CD).

β -CD molecular formula $C_{42}H_{70}O_{35}$ and molecular weight 1134.98. It has the melting point of 150 °C and soluble in 1 M NaOH (50mg/ml). The β -CD sugar molecules are connected together in the form of a ring (cyclic oligosaccharide) [1]. β -CD can be used as a complex agent to increase solubility, bioavailability and stability of poorly soluble drugs, Food, medicine, drug delivery, chemical industries, agricultural and ecological engineering. Crystal polymorphs have different soluble properties. Further warming is less soluble than the standard polymer lesser thermodynamic polymer. Pharmaceutical polymorphs vary in drugs such as shelf life, biochemistry, transformation, vapor pressure, density, color and compressibility [2-3].

Recommended solvent is water and solvate compound. Pharmaceutical drugs, some chemicals in the preparation of drugs for medical use. β -CD drugs are used to increase dissolution, drugs used in the treatment of acute rheumatic pain, rheumatic disease, osteoarthritis, and acute rheumatic pain.

This article discusses density, ultrasonic speeds, and THF displays with β -CD in water systems of sluggish mixture over the entire composition range at 303.15–313.15 K. From the tentative data, various physical parameters and areas of infinite dilution have been analyzed. As a result, bipolar-stimulus-bipolar interaction between the elements of the mixture, resulting in the formation of electron donor-acceptor complexes are studied in terms of molecular interactions.

MATERIAL AND METHODS

All the binary liquid mixtures were prepared by weighing all the binary liquid mixtures and the correct size of the fluids in a balanced bottle. The uncertainty of the electronic balance is ± 0.01 mg but the particle portion of the precision is $\pm 1 \times 10^{-4}$. An electronic-driven standard temperature to measure water by measurement of the required dual pressure, temperature measurement accuracy is 0.01 K.

The density of pure liquids and their compounds and the electrolytic solution are measured using a measurable measurement method using a 5 ml corning specific gravity bottle [4]. At the temperature of the test was measured in a specific gravity weighing twice as distilled water. By using the following contact, the density of the unknown mixture is determined at any given temperature.

$$\rho_s = (W_s/W_w \times \rho_w) \quad \text{“Eq.(1)”}$$

Where, ρ_w is the density of water, W_s and W_w are the weight of unknown solution and water respectively. The densities of pure liquids thus found are established to be in good agreement with the standard values.

An Ostwald’s viscometer (10 ml) is used to determine the viscosity of the purest liquid, liquid mixtures and electrolytes. The viscometer was filled with dissolved water, then immersed into the water bath, which was placed at temperatures. The time of water flow is indicated after the liquid within the temperature of the heat.

The water was replaced with a mixture of the mixture. The flow rate of the mixture is measured.

An Ostwald’s viscometer (10 ml) was used for the determination of viscosity for the pure liquid, liquid mixtures and electrolytes by relative method. The viscometer was filled with conductivity water and then immersed in the water bath, which was kept at the experimental temperature [5]. The time of flow of water was noted after the liquid inside the viscometer attained temperature. The water was replaced by the mixture whose viscosity is to be determined. The viscosity of the mixture can be determined using the relation,

$$\eta_s = \eta_w \frac{\rho_s t_s}{\rho_w t_w} \quad \text{“Eq. (2)”}$$

Where η_s and ρ_s are viscosity and density of the solution respectively. η_w and ρ_w are the corresponding values for water. The time of flow was measured with an accuracy of ± 0.1 ms. The density and viscosity measurements were carried out in a well-stirred water bath whose temperature can be controlled [6-7]. All measurements were made at a constant temperature with an accuracy of ± 0.1 °C since viscosity is highly temperature sensitive.

Ultrasonic speed measurements operated with an accuracy of ± 0.1 MS⁻¹ in an ultrasonic interferometer (model M 84, M/S Mittal Enterprises, New Delhi), T = 303.15-313.15 K. measuring cell of interferometer for temperature variables is a specially designed double-wall vessel. Digital electronic constant temperature bath operated in an electronic mode (Model SSI-03 Spl, provided by M / S Mittal Enterprises, New Delhi) to -10 ° C temperature range up to 85 ° C with an accuracy of ± 0.1 ° C is used to circulate water through the outer jacket of a double-wall measurement cell containing the test liquid.

RESULT AND DISCUSSION

The density, speed velocity and viscosity of the pure liquid mixtures of the different mole fractions of β -CD are given in Table 1. In the Table 1, Molar volumes and excess adiabatic compressibility, free volume, internal pressure, free length and relaxation time are provided with higher rating values. Table 2-3. These graphs are represented by a Figs. 1 respectively. Molar volume data is affected by (i) breaking hydrogen bonds and dipolar association loss, difference size and shape. Interconnected interaction between [8-10], (ii) unlike hydrogen bonding or donor-acceptor-related molecules. The previous effect leads to positive over-molar volumes, and the latter effect results in negative estimates. In this analysis suggest that negative values dominate the present investigation for all binary compounds in total incomplete range at T = (303.15 to 313.15) K.

Table 1. Measured values of density (ρ) of the pure liquids at 303.15 K.

Components	Density (ρ) Kg m ⁻³		References
	Observed Values	Literature Values	
THF	870	877.1	M. V. Rathnam et al. (2013). [5]
β -CD	996.2	999.6	A. Balcerzak et al. (2008). [25]

The excess volume has positive value for system of β -CD + THF + water at T = (303.15 to 313.15) K in the complete mixing range and in all experimental temperatures. The positive values of V^E indicated that absence of specific contacts, such as hydrogen bonding between the mixed components, dipole-dipole or dipole-dipole induced interaction, leads to electron donor-carrier complexes. Hydrogen bonding interaction (O-H ...) had greater efficiency between β -CD and THF in water.

Furthermore, an interaction between the possibility of the electron donor - β -CD and the electron donation of water. Such electron donation-accepting interactions act as the β -CD electron donor and THF action electron acceptor [11-15].

In the present study, interactions between β -CD and THF may result in dipole-induced-dipole interactions between the components of the mixtures as a result of the formation of electron donor-acceptor complexes. The Tetra hydro furan oxygen atom with β -CD in water, changes the bonds to expel the ring from a positive charges to the ring to the oxygen (mesmeric effect greater than inductive effect). However, this is donor-accepting complexes.

However, this is donor-accepting act [16-19]. As a result of these two adverse effects, the negative transfers to the oxygen atom from the ring, and expanding the acceptability of the THF. Therefore, the interchange between the THF with β -CD in water should be increased due to the connectivity of the oxygen and hydroxyl atom at the water through the β -CD.

Table 2. Measured values of density (ρ), ultrasonic velocity (U), viscosity (η) and Molar volume (V_m) for β -CD + THF + water at 303.15–313.15 K.

Mole fraction(X_2)	Density (ρ) Kg m^{-3}	Viscosity (η) $\times 10^3$ Nsm $^{-2}$	Ultrasonic velocity (U) ms $^{-1}$	Molar volume (V_m) m 3
System: β -CD + THF + water at 303.15 K				
0.1033	996.2	0.7073	1519	0.1821
0.1136	995.7	0.7106	1520	0.1932
0.1263	995.1	0.7202	1521	0.2068
0.1420	994.6	0.7326	1524	0.2237
0.1623	993.7	0.7485	1527	0.2456
System: β -CD + THF + water at 308.15 K				
0.1033	993.8	0.7473	1528	0.1825
0.1136	992.7	0.7491	1529	0.1938
0.1263	991.1	0.7502	1531	0.2076
0.1420	990.6	0.7513	1532	0.2246
0.1623	989.7	0.7529	1533	0.2466
System: β -cyclodextrin + THF + water at 313.15K				
0.1033	989.8	0.7530	1534	0.1833
0.1136	988.7	0.7538	1537	0.1946
0.1263	987.1	0.7542	1545	0.2084
0.1420	986.6	0.7556	1549	0.2255
0.1623	985.7	0.7568	1558	0.2476

Table 3. Calculated values of Excess free volume, internal pressure, adiabatic compressibility, free length and relaxation time of β -CD + THF + water at 303.15–313.15K.

Mole fraction (X_2)	Excess Free volume (V_F^E) $\times 10^7$ $\text{m}^3 \text{mol}^{-1}$	Excess Internal pressure (π_i^E) $\times 10^7$ Nm^{-2}	Excess Adiabatic compressibility (β^E) $\times 10^{10}$ Pa^{-1}	Excess Free length (L_F^E) $\times 10^{10}$ m	Excess Relaxation time (τ^E) $\times 10^{-5}$ s
System: β -CD + THF + water at 303.15 K					
0.1033	0.1228	-0.3524	5.0805	-0.4177	0.1116
0.1136	0.1350	-0.3878	5.5878	-0.4594	0.1227
0.1263	0.1499	-0.4310	6.2080	-0.5103	0.1363
0.1420	0.1685	-0.4850	6.9833	-0.5741	0.1534
0.1623	0.1925	-0.5543	7.9800	-0.6560	0.1752
System: β -CD + THF + water at 308.15 K					
0.1033	0.1140	-0.3602	5.0480	-0.4190	0.1184
0.1136	0.1253	-0.3964	5.5520	-0.4608	0.1302
0.1263	0.1391	-0.4406	6.1682	-0.5120	0.1446
0.1420	0.1564	-0.4958	6.9384	-0.5759	0.1627
0.1623	0.1786	-0.5667	7.9286	-0.6581	0.1859
System: β -CD + THF + water at 313.15 K					
0.1033	0.1147	-0.3644	4.9769	-0.0536	0.1195
0.1136	0.1260	-0.4010	5.4740	-0.0590	0.1314
0.1263	0.1399	-0.4457	6.0818	-0.0655	0.1460
0.1420	0.1573	-0.5015	6.8413	-0.0737	0.1642
0.1623	0.1796	-0.5733	7.8180	-0.0842	0.1876
Mole fraction (X_2)	Excess Free volume (V_F^E) $\times 10^7$ $\text{m}^3 \text{mol}^{-1}$	Excess Internal pressure (π_i^E) $\times 10^7$ Nm^{-2}	Excess Adiabatic compressibility (β^E) $\times 10^{10}$ Pa^{-1}	Excess Free length (L_F^E) $\times 10^{10}$ m	Excess Relaxation time (τ^E) $\times 10^{-5}$ s
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Table 4. Calculated values of cohesive forces, Auerbach relation (σ_{Auer}) modified relation (σ_{Mod}) of β -CD + THF + water at 303.15–313.15 K.

Mole fraction X_2	Cohesive forces 10^6 kJ mol^{-1}	Auer Bach relation (σ_{Auer}) m N/m	Modified relation (σ_{Mod}) m N/m
System: β -CD + THF + water at 303.15K			
0.1033	610715.90	1108.2	111988.6
0.1136	612254.70	1111.0	112266.2
0.1263	616102.84	1113.9	112555.8
0.1420	620849.39	1121.0	113280.0
0.1623	627159.78	1128.7	114053.5
System: β -CD + THF + water at 308.15K			
0.1033	636731.42	1130.8	116150.9
0.1136	637518.34	1134.3	116508.0
0.1263	637930.02	1140.6	117154.7
0.1420	638276.95	1143.4	117443.6
0.1623	638940.85	1146.7	117780.8
System: β -CD + THF + water at 313.15K			
0.1033	649137.23	1148.8	119914.1
0.1136	649088.35	1156.8	120753.2
0.1263	647927.13	1176.9	122847.4
0.1420	647799.72	1186.7	123866.8
0.1623	646635.35	1208.6	126153.5

Mole fraction (X_2)	Excess Free volume (V_F^E) $\times 10^7$ $\text{m}^3 \text{mol}^{-1}$	Excess Internal pressure (π_i^E) $\times 10^7$ Nm^{-2}	Excess Adiabatic compressibility (β^E) $\times 10^{10}$ Pa^{-1}	Excess Free length (L_F^E) $\times 10^{10}$ m	Excess Relaxation time (τ^E) $\times 10^{-5}$ s
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V^E data showed a more positive excess volume values than the previous one in Table 3 for the ternary systems of Tetra hydro furan with β -CD in water. The electron reverses the hydroxyl group (negative stimulus effect) in the β -CD ring. But the electron density of the THF ring decreases. As a result, the electron donation on behalf of THF electron [20-22].

Mole fraction (X_2)	Excess Free volume (V_F^E) $\times 10^7$ $\text{m}^3 \text{mol}^{-1}$	Excess	Excess Adiabatic compressibility (β^E) $\times 10^{10}$ Pa^{-1}	Excess Free length (L_F^E) $\times 10^{10}$ m	Excess Relaxation time (τ^E) $\times 10^{-5}$ s
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0.1623	0.1796	-0.5733	7.8180	-0.0842	0.1876

Tetra hydro furan with β -CD in water may have positive V^E data due to the low dipolar moment and dielectric constant. THF should be a relatively complex molecule and its oxygen group rotates freely in the C-N axis, which provides more flexibility for contact with β -CD in water.

At higher temperatures, V^E values increases may be due to factors (i) at higher temperatures, a set of components, (ii) dipole-dipole interactions have been weakened and (iii) increases the kinetic energy.

The excess isentropic compressibility data are given in Table 3 and on the table. 1. The study of data in the Table 3, the excess isentropic compressibility data of the highest equation for these systems in the total system range at 303.15-313.15 K.

The first factor influence positive values, whereas the remaining two factors indicated to negative values [23]. The positive values for this system indicates that the system is more compressible.

The sign of viscosity depends on the size, shape, and internal strategic forces [24-25]. Positive values of viscosity shows that the viscosity of the pure mixture is higher than the β -CD in water systems for Tetra hydro furan, so the mixture is less fluid.

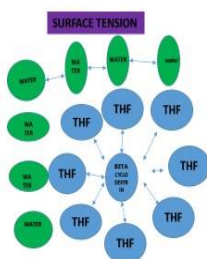
This refers to the existence of specific interaction rather than unlike molecules, such as the electron donor-acceptor. Viscosity deviation values resemble molar volumes for this system.

Because the molar volumes of each in the mixture is less than the molar volume in the pure state, due to the creation of electron donor-acceptor, there is a contraction in volume mixing.

However, as temperature increases and becomes more negative, there are enhanced solute -solvent interactions between molecules within β -CD with water molecules in THF.

The Cohesive data are given in Table 4 and graphically presented in Fig. 2. The Cohesive values are found to be increased over the entire composition range at T= (303.15 to 313.15) K Tetra hydro furan with β -CD in water system.

Estimated values can be described as standard, by considering cohesive forces between water liquid between THF molecules, which are shared with neighboring molecules of β -CD. There is no neighboring approach and stronger attractive forces are exposed to their neighbors on the surface. This attractive expansion on the surface of the Tetra Hydro Furan with the β -CD in water system.

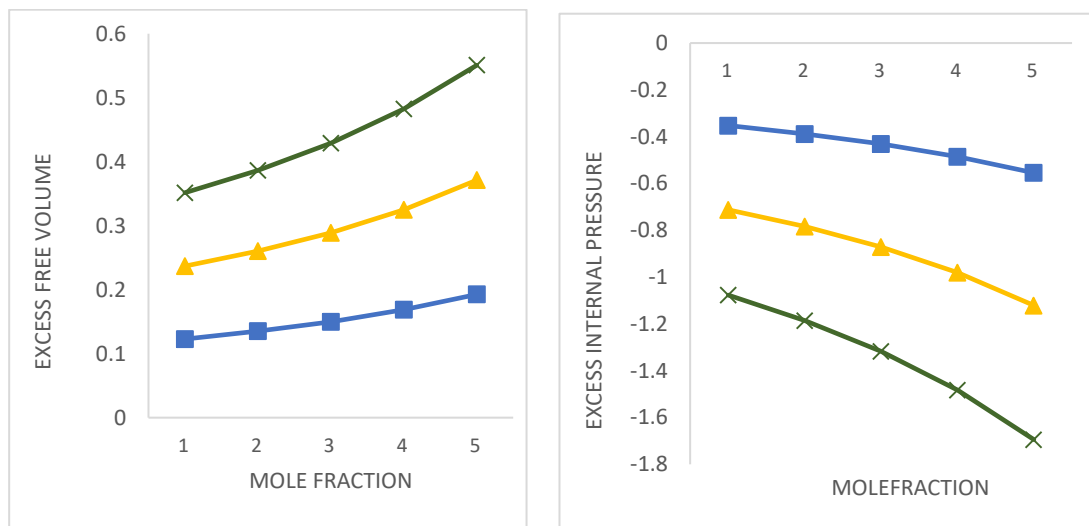


The observed values of surface tension is given in Table 4 and graphically presented in Fig. 2. The surface tension are found to be increased over the entire composition range at $T = (303.15-313.15)$ K, THF with β -CD in water system by using Auerbauch relation and modified relations.

Molecular fluid state have strong intermolecular attractive forces. When these forces are between like molecules, they are referred to as cohesive forces. The water molecules in water are associated with the β -CD in the water system in the surface of the THF, especially by strong cohesive forces.

When attractive forces are unlike molecules, those molecules are said to be adhesive forces. The resin forces between water molecules and β -CD walls with THF are stronger than cohesive force leads to contribute capillary actions. These fascinating forces between the β -CD with THF in water systems can be seen by the remaining electrostatic and van der Waal's forces.

Fig. 1. Plots of excess volume of free volume, adiabatic compressibility, internal pressure, free volume and relaxation time for various mole fractions of β -CD + THF + water at 303.15-313.15 K.



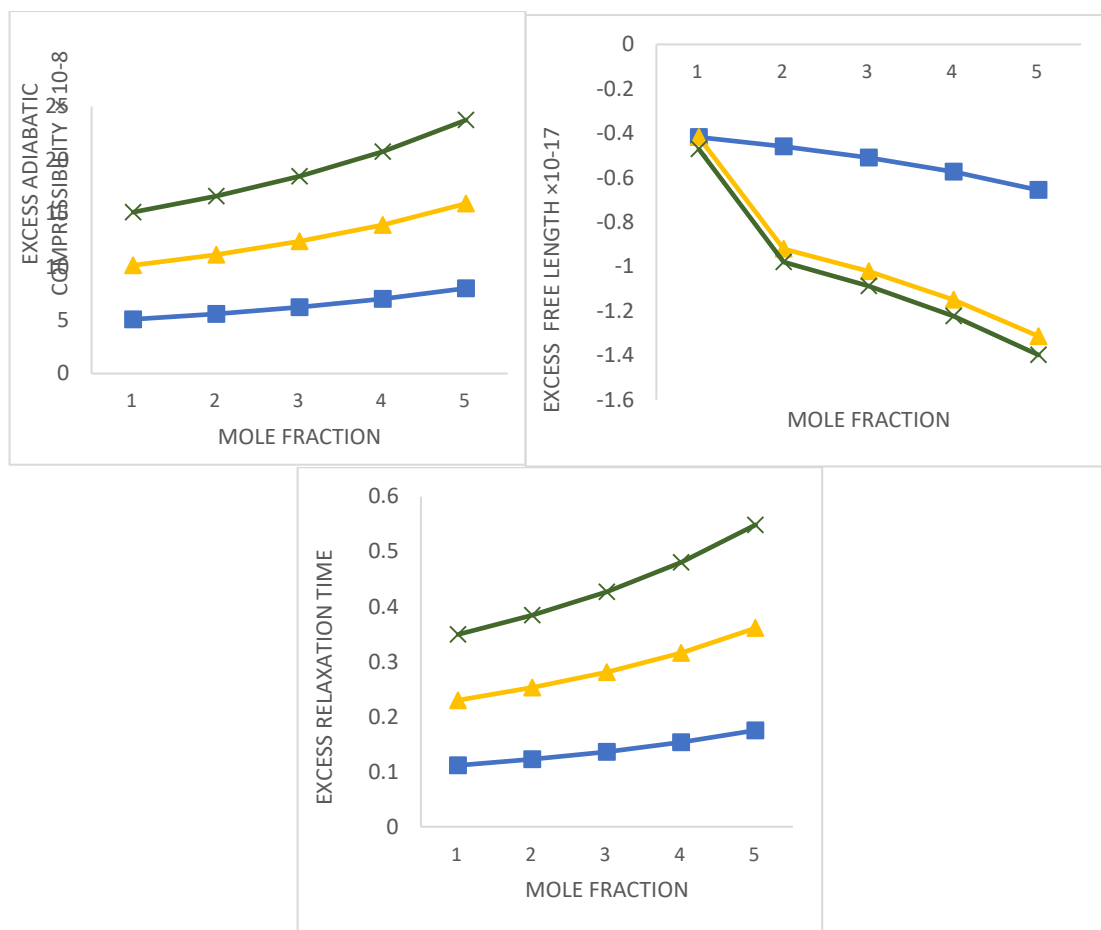
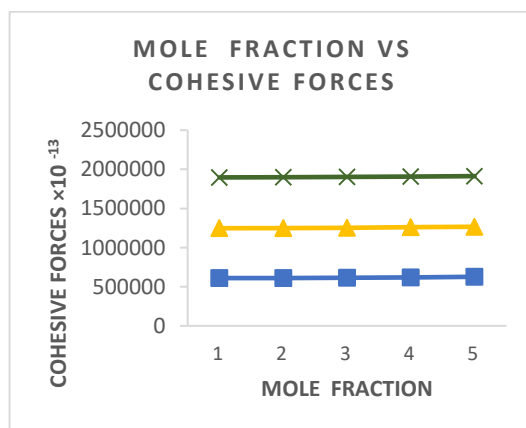
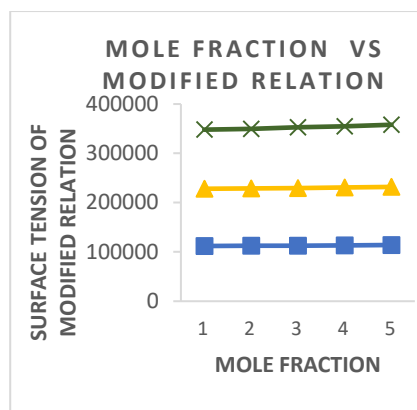
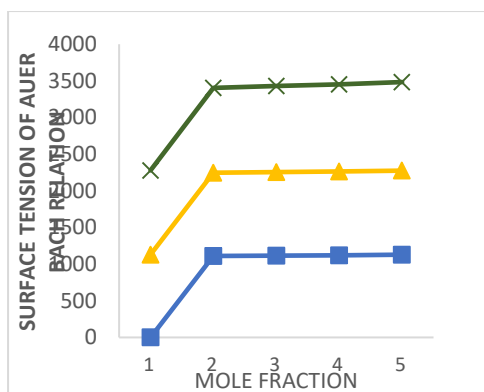


Fig. 2. Plots of cohesive force, surface tension of Auer Bach relation, and surface tension of modified relation, for various mole fractions of β -CD + THF + water at 303.15-313.15K.





CONCLUSIONS

This paper reports the densities, speeds of sound and viscosities of THF with β -CD in water system of ternary mixtures on the whole composition series at 303.15 to 313.15K. The values of pure components generally support available literature data. Many physicochemical parameters of infinite dilution components are assessed from tentative data, which are analyzed on molecular interactions on dipole-induce-dipole interactions between the components of the mixtures, resulting in electron donations acceptable premises. The lower spread of the THF interface in the β -CD (long hydrophobic tail) water containing a high molecular mass and tightly adsorbed to the interface by functioning a cohesive force on the surface, resulting in tetra hydro furan surface tension with the β -CD water system. Consequently, strong molecular interaction between adjacent molecules affecting strong surface film face on THF with β -CD in water system at higher concentration.

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List of symbols

K_T : Temperature dependent constant
 M : Molality
 ρ : Density
 η : Viscosity
 U : Ultrasonic velocity
 V_m : Molar volume
 β^E : Excess adiabatic compressibility
 V_F^E : Excess free volume
 L_F^E : Excess free length
 π_i^E : Excess internal pressure
 σ_{Auer} : Surface tension of Auer bauch Relation
 σ_{Mod} : Surface tension of Modified Relation
 β -CD: Beta Cyclodextrin

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