

Transport Properties of Vitamin B₃ in Aqueous Mixtures Of d-Fructose

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Abstract:

The viscosity of vitamin B₃ in water and in different solutions of D-fructose (D-fru) in water at different temperatures has been determined. To calculate A and B parameter of Jones Dole equation experimental values of relative viscosities were used. Feakin's Transition-State Theory was used to determine the activation parameters. Results have been concluded in the form of molecular interactions and structure behavior of vitamin B₃ in water and aqueous solutions of D-fructose.

Keywords: Viscosity B - parameter, structure maker and relative viscosity.

1. Introduction

In the physical chemistry transport properties are considered to be more efficient in giving the details of interactions occurring in the solution. Viscometric study is one of the transport study conducted to gather knowledge about physical properties and structural variation in the solutions [1-3]. There are various types of molecular interactions occur in solutions out of which interaction between solute and solute, solute and solvent are the one which play a major role. Structure making and breaking behaviour of solute can also be predicted by using these interactions. As per literature it was found that many studies have been conducted on various electrolytes, non-electrolytes and biomolecules but out of these, biomolecules are the current area of interest [4-15]. It is also found that a lot of studies were already conducted over number of biomolecules found in nature but less attention was given to the transport properties of vitamin B₃ in aqueous medium and different concentrations of D-fru in water. Vitamin B₃ is an important component in pharmacological doses and plays the major role in production of steroid hormones and DNA repairing. The fructose is commonly used as the part

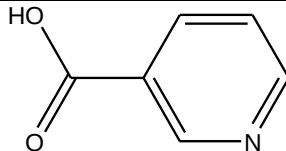
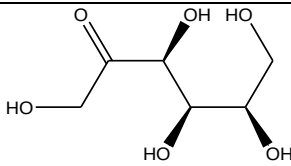
of our diet and also used as an alternate for sugar. Therefore, it is necessary to study the molecular nature of vitamin B₃ in the binary solutions of fructose.

2. Experimental

2.1 Material

The chemicals used in the study have been used without further purification and were purchased from S.D Fine-Chem. Limited. The details for the same are mentioned in Table number 1.

Table number 1: Details of chemicals utilized in study.

Name of Chemical	Purity [#]	Structure
Vitamin B ₃ (Nicotinic acid)	>0.99	
D-fructose	>0.99	

As stated by supplier

2.2 Methods

All the solutions and compositions were prepared by using the double distilled deionized water having a pH of 7.1. The analytical balance (FA2204B) was used for preparing the molal solutions with an uncertainty of ± 0.0001 g. A density analyzer (Anton Paar DSA 5000) was used to determine the respective densities of the solutions. The values of the densities were further utilized to determine the relative viscosities. A suspended level viscometer in water thermostat (± 0.001 K) [16-17] was used to determine the time flow for the solutions which were further used in calculating the relative viscosities using the following relation:

$$\eta_{\text{rel}} = \frac{\eta}{\eta_0} = \frac{t \rho}{t_0 \rho_0} \quad (1) \text{ Here } \eta,$$

η_0 , ρ and ρ_0 are the respective viscosities and densities whereas t and t_0 are the flow time of solution and solvent.

3. Results and Discussion

From the obtained data of respective viscosities, it is clear that the obtained values of viscosities rise in magnitude with an increment in concentration of vitamin B₃ in the solutions with an increment in compositions of D-fruand also with increase of temperature (298.15 to 318.15) K.

The obtained data of relative viscosity has been interpreted with Jones-Dole equation[18].

$$\eta_{rel} = \frac{\eta}{\eta_0} = 1 + AC^{1/2} + BC \quad (2)$$

here, the *A* parameter and *B* parameters correspond to the molecular interactions. *A* parameter corresponds for the molecular interaction between solute and solute whereas *B* corresponds for interaction between solute and solvent. It is found that molecular action of vitamin B₃ is same for all the different composition of D-fruin water. The values of *A* parameter and *B* parameter in various compositions of D-fruin water at 30°C are represented in the table number 2 and the respective graph of $(\eta_r - 1)/c^{1/2}$ vs. $c^{1/2}$ of vitamin B₃ in all the different concentrations of D-fruin water at 303.15 K is shown in graph 1.

TABLE 2. Jones – Dole parameters for vitamin B₃ in various compositions of D-fruin water at 303.15K.

<i>m</i>	<i>A</i> / m ^{3/2} mol ^{-1/2}	<i>B</i> / m ³ mol ⁻¹
0.05	4.243 (±0.309)	0.382 (±0.011)
0.15	4.212(±0.191)	0.390(±0.007)
0.25	4.148(±0.214)	0.399(±0.008)
0.35	4.116(±0.171)	0.407(±0.006)

m denotes the molal concentration of D-fruin water in mol.kg⁻¹

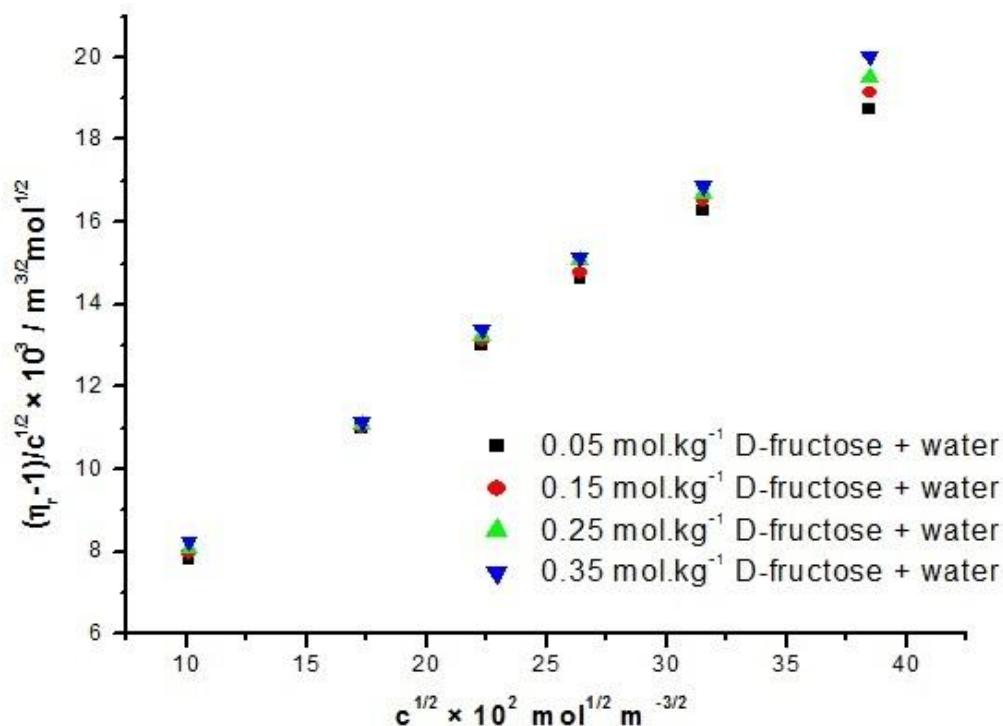


Fig 1: Graph of $(\eta_r-1)/c^{1/2}$ vs $c^{1/2}$ vitamin B₃ in various compositions of D-fru in water at 303.15 K

From Table number 2, the A-parameter values are showing decrement with the rise in compositions of D-fruin water which indicates the decrement in the solute-solute interactions. Also it is found that the values of B-parameter are rising with the rise in concentration of D-fruin water at 303.15 K, thereby indicating the strengthening of solute – solvent interactions.

The theory given by Feakinset.al[19] is used for the analyses of data by using the following relation:

$$B = \frac{\overline{V}_1^0 - \overline{V}_2^0}{1000} + \frac{\overline{V}_1^0}{1000} \left[\frac{\Delta\mu_2^0 - \Delta\mu_1^0}{RT} \right] (3)$$

Where,

$\overline{V}_1^0$ denotes mean volume of the pure solvent, $\overline{V}_2^0$ denotes the partial molar volume for vitamin B₃. $\Delta\mu_1^{0*}$ denotes the free energies of activations for the pure solvent, $\Delta\mu_2^{0*}$ denotes the free energies of activations for the solution.

The values of $\Delta\mu_1^{0*}$ and $\Delta\mu_2^{0*}$ are framed using following relations [20]:

$$\Delta\mu_1^{0*} = RT \ln \left(\eta_0 \bar{V}_1^0 / hN \right) \quad (4)$$

$$\Delta\mu_2^{0*} = \Delta\mu_1^{0*} \ln RT / \bar{V}_1^0 \left[1000B - (\bar{V}_1^0 - \bar{V}_2^0) \right] \quad (5)$$

Where,

h denotes Planck's constant, η_0 denotes viscosity of the solvent, T denotes absolute temperature, N denotes Avogadro number, R denotes the universal gas constant.

The values obtained using above equation 4 are given in Table 3. The data of density is used to determine the values of $\bar{V}_2^0$ (partial molar volumes). Table 3 represents the values of $\Delta\mu_1^{0*}$, $\Delta\mu_2^{0*}$ which were determined by using above equation number (4) and (5).

TABLE 3: $\bar{V}_1^0$, $\bar{V}_2^0$, $\Delta\mu_1^{0*}$ and $\Delta\mu_2^{0*}$ parameters for vitamin B₃ in various composition of D-fru in water at 303.15 K.

m	$\bar{V}_1^0 \times 10^3$ / m ³ mol ⁻¹	$\bar{V}_2^0 \times 10^3$ / m ³ mol ⁻¹	$\Delta\mu_1^{0*}$ / kJ mol ⁻¹	$\Delta\mu_2^{0*}$ / kJ mol ⁻¹
0.05	18.15	81.41	26.66	61.87
0.15	18.31	81.94	26.72	62.46
0.25	18.48	82.18	26.77	63.13
0.35	18.67	82.61	26.82	63.61

m denotes the molality of D-fru in water in mol.kg⁻¹

The data in Table 3 reports the mean volume of the solvent i.e. $\bar{V}_1^0$ which are found to be invariable and are not affected by varying the concentration of D-fru in water at the 303.15K. The values of $\Delta\mu_2^{0*}$ were found increasing with the increases in the composition D-fru in water at the temperature of 303.15K indicating the formation of transition state and resulting in distortions and making of the molecular bonds between water and molecules of D-fructose.

Effect of temperature

The molecular behavior of vitamin B₃ was found to be similar in the different concentrations of D-fru in water at the temperature 303.15 K. So, the 0.05 mol.kg⁻¹ D-fru in water (the lowest composition) has been chosen to interpret the consequence of temperature. The graph of $(\eta_r -$

$1)/c^{1/2}$ vs. $c^{1/2}$ for vitamin B₃ in water and 0.05 mol.kg⁻¹ D-fru in water at different temperatures are shown in figure number 2 and 3.

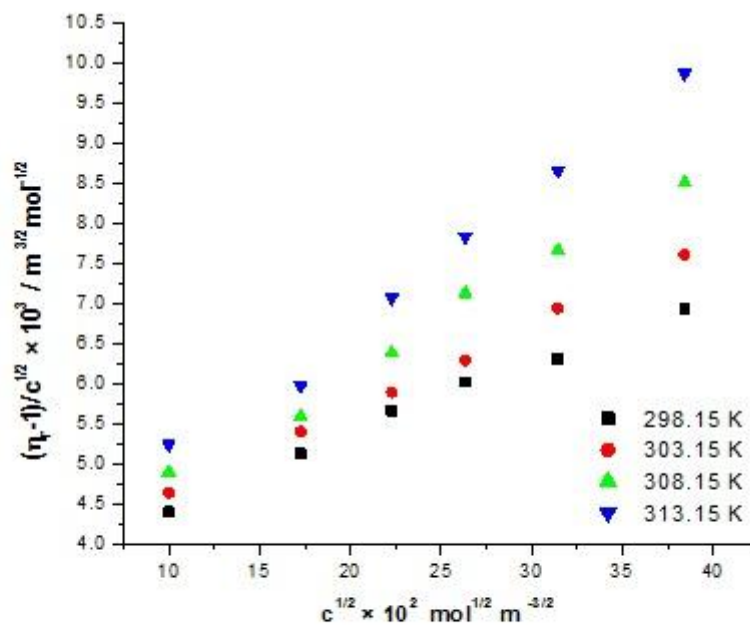


Fig 2: Graph of $(\eta_r - 1)/c^{1/2}$ vs $c^{1/2}$ for vitamin B₃ in water at different temperature.

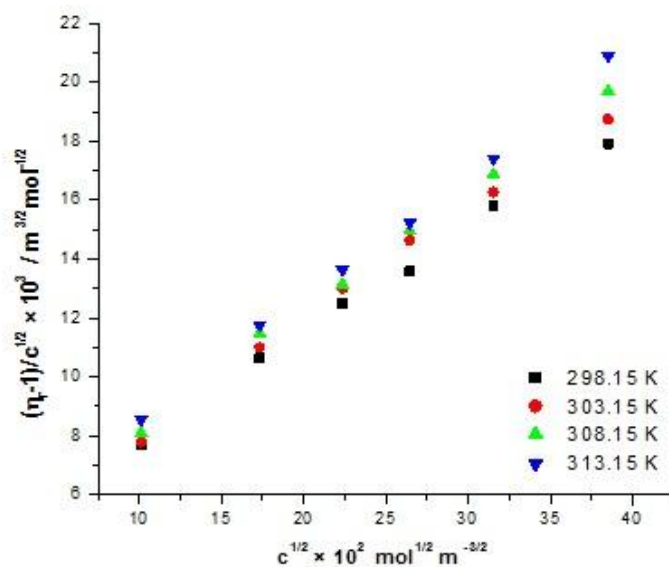


Fig 3: Graph of $(\eta_r - 1)/c^{1/2}$ vs $c^{1/2}$ for vitamin B₃ in 0.05 mol.kg⁻¹ D-fru in water at different temperature.

Table 4: Jones – Dole A and B parameters for vitamin B₃ in water, D-fru in water at five equidistant temperatures.

Temperature / (K)	A / (m ^{3/2} .mol ^{-1/2})	B / (m ³ .mol ⁻¹)
Water		
298.15	3.601(±0.059)	0.088(±0.002)
303.15	3.575(±0.048)	0.105(±0.001)
308.15	3.491(±0.157)	0.132(±0.006)
313.15	3.353(±0.209)	0.169(±0.008)
0.05 mol.kg⁻¹ D-fru in water		
298.15	4.261(±0.272)	0.359(±0.010)
303.15	4.243(±0.309)	0.382(±0.011)
308.15	4.218(±0.216)	0.403(±0.008)
313.15	4.192(±0.275)	0.427(±0.010)

It has been found from the table number 4 that the A –Parameter values for vitamin B₃ in water and in 0.05 mol.kg⁻¹ D-fru in water decreases with increase in temperature clarifying the decrease of interactions between molecules of solute and solvent with the increment of temperature. Also the B-parameter values are increasing with the rise in temperature suggesting the increase of solute-solvent interactions with increase of temperature and also leads to structure breaking behavior of vitamin B₃ in aqueous medium as well as in binary aqueous mixtures of D-fru. The Feakin's transition state theory is used to interpret the viscosity data at different temperatures and further used to calculate values of $\Delta\mu_1^{0*}$ and $\Delta\mu_2^{0*}$ that have been represented in table number 5.

TABLE 5: $\overline{V}_1^0$, $\overline{V}_2^0$, $\Delta\mu_1^{0*}$ and $\Delta\mu_2^{0*}$ values for vitamin B₃ in 0.05 mol.kg⁻¹ D-fru in water at different temperatures.

Temperature / K	$\overline{V}_1^0 \times 10^3$ / m ³ mol ⁻¹	$\overline{V}_2^0 \times 10^3$ / m ³ mol ⁻¹	$\Delta\mu_1^{0*}$ / kJ mol ⁻¹	$\Delta\mu_2^{0*}$ / kJ mol ⁻¹
298.15	18.12	80.45	26.34	57.67

303.15	18.15	81.41	26.66	61.87
308.15	18.18	81.76	26.99	65.80
313.15	18.21	83.03	27.32	70.35

TABLE 6: ($\Delta\mu_2^{0*}-\Delta\mu_1^{0*}$), $T\Delta S_2^{0*}$ and ΔH_2^{0*} values for vitamin B₃ in 0.05mol.kg⁻¹D-fru in water at five equidistant temperatures.

T / K	$\Delta\mu_2^{0*}-\Delta\mu_1^{0*}$ / (kJ mol ⁻¹)	$T. \Delta S_2^{0*}$ / (kJ mol ⁻¹)	ΔH_2^{0*} / (kJ mol ⁻¹)
298.15	31.33	-250.15	-192.48
303.15	35.21	-254.34	-192.47
308.15	38.81	-258.54	-192.74
313.15	43.03	-262.73	-192.38

The values of ($\Delta\mu_2^{0*}-\Delta\mu_1^{0*}$) are found to be positive and large and are recorded in table number 6 supporting that the presence of vitamin B₃ is favoring the transition state for the complete temperature range. The ΔS_2^{0*} values are obtained from the values of slopes of the linear graphs of $\Delta\mu_2^{0*}$ vs temperature by using following equation:

$$\frac{d(\Delta\mu_2^{0*})}{dT} = -\Delta S_2^{0*} \quad (6)$$

The data of enthalpy of activation i.e. ΔH_2^{0*} are obtained using following equation [19]:

$$\Delta H_2^{0*} = \Delta\mu_2^{0*} + T. \Delta S_2^{0*} \quad (7)$$

The $T. \Delta S_2^{0*}$ and ΔH_2^{0*} values are represented in the table 6. The negative values of entropy and enthalpy of activation of vitamin B₃ in various composition of D-fru at different temperatures indicates increase in order and bond making is associated by transition state theory [20-21].

4. Conclusion

The study concludes that the vitamin B₃ acts as structure maker in both water and different compositions of D-fructose and the increase in order and bond making is associated by transition state theory.

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