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Structural effects of three carbohydrates in nicotinic acid/water mixed solvents

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ABSTRACT

Density (ρ) and viscosity (η) measurements of bio-active solutes (D-glucose, D-mannitol and D-sucrose) in aqueous nicotinic acid, (Vitamin B_3) at 298.15, 308.15 and 318.15 K have been carried out. Using these properties, the apparent molar volume (ϕ_V), the partial molar volume (ϕ_V^0), the partial molar volume of transfer ($\Delta\phi_V^0$) of carbohydrates from water to aqueous nicotinic acid solution were calculated. A plausible mechanism for the reaction of carbohydrates in aqueous nicotinic acid is also suggested along with the interaction of the product with water. The viscosity *B*-coefficients of Jones–Dole equation and the molar refraction (R) of the solutions have been computed for the interpretation of solute–solvent interactions. The structure-making or breaking capacity of carbohydrates in the solution has been discussed. All these parameters are used to study solute–solvent and solute–solute interactions in the aforementioned mixtures.

1. Introduction

Carbohydrates (bio-active solutes) are the most abundant class of organic compounds found in living organism. They perform numerous roles in living system for the storage and transport of energy to participation in immune-system. Understanding their behaviour in dilute solutions is of utmost importance in medicinal and biological systems. The pyridine-monocarboxylic acids are examples of amphiprotic [1] electrolytes that are of considerable biological interest. Nicotinic acid (3-pyridine carboxylic acid), also known as niacin or pellagra-preventing factor, is an important compound which play a crucial role in various physiological effects, biosynthesis, metabolic reactions, and several drug preparations [2]. The physicochemical and thermodynamic properties of nicotinic acid are of considerable interest as it is an essential nutrient for humans and certain other animal species, in which it functions as a vitamin. Studies on densities, viscosities, and refractive indices of studied solutions are of great use in characterizing the structure and properties of solutions. Various types of interactions exist between the solutes in solutions, as solute–solute and solute–solvent interactions [3,4] provide a better understanding of the nature of the non-electrolytes in solution, which is very significant to investigate their physicochemical behaviour. Among various physical parameters, these thermodynamic parameters have been recognised as being sensitive to structural changes occurring in solutions. Moreover, model compound studies have been necessitated owing to the complex structural organisation of the biological macromolecules.

In this article, an attempt has been made to reveal the nature of various types of interactions prevailing in carbohydrates (D-glucose, D-mannitol and D-sucrose) in $w_1 = 0.005, 0.01, 0.015$ mass fraction of aqueous nicotinic acid (NA) binary mixtures at 298.15, 308.15, and 318.15 K from volumetric, viscometric and refractometric measurements. The aim of the present work is to study the molecular interactions of carbohydrates in aqueous solutions of nicotinic acid by physicochemical and thermodynamical studies, and the structural effect of carbohydrates as literature survey reveals that very scarce work has been carried out in the present ternary systems. Such study helps in better understanding of the interactions occurring between

Table 1
Values of density (ρ), viscosity (η), at 298.15, 308.15, 318.15 K and refractive index (n_D) at 298.15 K in different mass fractions (w_1) of aqueous NA.

Mass fraction of aq NA (w_1)	Temp/K[a]	$\rho \cdot 10^{-3}$/kg m^{-3}[b]	η/mPa s[c]	n_D[d]
$w_1 = 0.005$	298.15	0.99742	0.891	1.3320
	308.15	0.99431	0.720	–
	318.15	0.99047	0.584	–
$w_1 = 0.010$	298.15	0.99750	0.893	1.3323
	308.15	0.99448	0.721	–
	318.15	0.99062	0.587	–
$w_1 = 0.015$	298.15	0.99767	0.895	1.3328
	308.15	0.99465	0.722	–
	318.15	0.99081	0.589	–

[a] Uncertainty in temperature values ±0.01 K.
[b] Uncertainty in density values ±0.00005 g·cm^{-3}.
[c] Uncertainty in viscosity values ±0.003 mPa·s.
[d] Uncertainty in refractive index values ±0.0002 units.

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Table 2
Experimental values of density (ρ) and viscosity (η) at 298.15 K, 308.15 K, 318.15 K and refractive index (n_D) at 298.15 K of carbohydrates in different mass fractions of aqueous NA (w_1).

m/mol kg^{-1}[a]	$\rho \cdot 10^{-3}$/kg cm^{-3}	η/mPa s	n_D	m/mol kg^{-1}	$\rho \cdot 10^{-3}$/kg cm^{-3}	η/mPa s	n_D
$w_1 = 0.005$							
D-Glucose + aq. NA							
$T = 298.15$ K				$T = 298.15$ K			
0.0100	0.99801 ± 0.00001	0.893 ± 0.001	1.3324 ± 0.0002	0.0555	1.00128 ± 0.00002	0.909 ± 0.001	1.3343 ± 0.0001
0.0251	0.99902 ± 0.00001	0.898 ± 0.001	1.3330 ± 0.0002	0.0707	1.00252 ± 0.00003	0.915 ± 0.002	1.3350 ± 0.0001
0.0403	1.00012 ± 0.00002	0.904 ± 0.002	1.3336 ± 0.0001	0.0860	1.00379 ± 0.00002	0.921 ± 0.002	1.3357 ± 0.0001
$T = 308.15$ K				$T = 308.15$ K			
0.0101	0.99484 ± 0.00002	0.722 ± 0.002		0.0557	0.99793 ± 0.00002	0.737 ± 0.003	
0.0252	0.99578 ± 0.00001	0.727 ± 0.001		0.0710	0.99912 ± 0.00002	0.742 ± 0.002	
0.0404	0.99682 ± 0.00003	0.732 ± 0.002		0.0863	1.00038 ± 0.00003	0.747 ± 0.002	
$T = 318.15$ K				$T = 318.15$ K			
0.0101	0.99095 ± 0.00001	0.586 ± 0.001		0.0559	0.99393 ± 0.00004	0.599 ± 0.002	
0.0253	0.99183 ± 0.00003	0.590 ± 0.003		0.0712	0.99511 ± 0.00003	0.604 ± 0.002	
0.0406	0.99283 ± 0.00002	0.595 ± 0.001		0.0866	0.99639 ± 0.00002	0.609 ± 0.003	
D-Mannitol + aq. NA							
$T = 298.15$ K				$T = 298.15$ K			
0.0100	0.99803 ± 0.00003	0.894 ± 0.001	1.3326 ± 0.0001	0.0555	1.00147 ± 0.00003	0.915 ± 0.001	1.3346 ± 0.0002
0.0251	0.99907 ± 0.00001	0.901 ± 0.001	1.3332 ± 0.0001	0.0707	1.00278 ± 0.00004	0.922 ± 0.002	1.3353 ± 0.0001
0.0403	1.00023 ± 0.00002	0.908 ± 0.003	1.3339 ± 0.0001	0.0860	1.00420 ± 0.00002	0.931 ± 0.001	1.3361 ± 0.0002
$T = 308.15$ K				$T = 308.15$ K			
0.0101	0.99487 ± 0.00001	0.723 ± 0.002		0.0557	0.99820 ± 0.00002	0.742 ± 0.002	
0.0252	0.99587 ± 0.00001	0.729 ± 0.003		0.0710	0.99949 ± 0.00005	0.748 ± 0.003	
0.0404	0.99699 ± 0.00001	0.735 ± 0.001		0.0863	1.00089 ± 0.00004	0.755 ± 0.002	
$T = 318.15$ K				$T = 318.15$ K			
0.0101	0.99099 ± 0.00003	0.587 ± 0.001		0.0559	0.99418 ± 0.00003	0.603 ± 0.001	
0.0253	0.99194 ± 0.00002	0.592 ± 0.002		0.0713	0.99544 ± 0.00002	0.609 ± 0.001	
0.0406	0.99302 ± 0.00004	0.597 ± 0.001		0.0867	0.99678 ± 0.00002	0.615 ± 0.001	
D-Sucrose + aq. NA							
$T = 298.15$ K				$T = 298.15$ K			
0.0101	0.99870 ± 0.00004	0.896 ± 0.002	1.3330 ± 0.0001	0.0560	1.00522 ± 0.00002	0.931 ± 0.002	1.3365 ± 0.0001
0.0253	1.00078 ± 0.00005	0.907 ± 0.002	1.3341 ± 0.0002	0.0714	1.00757 ± 0.00004	0.943 ± 0.002	1.3378 ± 0.0002
0.0406	1.00296 ± 0.00003	0.919 ± 0.003	1.3353 ± 0.0001	0.0870	1.00999 ± 0.00002	0.955 ± 0.001	1.3391 ± 0.0001
$T = 308.15$ K				$T = 308.15$ K			
0.0101	0.99549 ± 0.00002	0.725 ± 0.001		0.0560	1.00165 ± 0.00002	0.754 ± 0.002	
0.0253	0.99743 ± 0.00001	0.734 ± 0.002		0.0714	1.00390 ± 0.00003	0.765 ± 0.003	
0.0406	0.99950 ± 0.00003	0.744 ± 0.002		0.0870	1.00620 ± 0.00004	0.776 ± 0.001	
$T = 318.15$ K				$T = 318.15$ K			
0.0101	0.99160 ± 0.00004	0.589 ± 0.002		0.0562	0.99758 ± 0.00002	0.614 ± 0.002	
0.0254	0.99347 ± 0.00003	0.597 ± 0.002		0.0717	0.99978 ± 0.00004	0.623 ± 0.002	
0.0407	0.99547 ± 0.00003	0.605 ± 0.003		0.0874	1.00203 ± 0.00003	0.632 ± 0.001	
$w_1 = 0.010$							
D-Glucose + aq. NA							
$T = 298.15$ K				$T = 298.15$ K			
0.0100	0.99807 ± 0.00003	0.895 ± 0.001	1.3326 ± 0.0001	0.0555	1.00131 ± 0.00002	0.912 ± 0.001	1.3346 ± 0.0002
0.0251	0.99906 ± 0.00002	0.900 ± 0.002	1.3332 ± 0.0001	0.0707	1.00254 ± 0.00004	0.918 ± 0.001	1.3353 ± 0.0001
0.0403	1.00015 ± 0.00001	0.906 ± 0.001	1.3339 ± 0.0001	0.0860	1.00381 ± 0.00003	0.924 ± 0.002	1.336 ± 0.0002
$T = 308.15$ K				$T = 308.15$ K			
0.0101	0.99496 ± 0.00001	0.723 ± 0.002		0.0557	0.99796 ± 0.00001	0.738 ± 0.003	
0.0252	0.99585 ± 0.00001	0.728 ± 0.001		0.0710	0.99914 ± 0.00002	0.744 ± 0.002	
0.0404	0.99686 ± 0.00002	0.733 ± 0.003		0.0863	1.0004 ± 0.00001	0.750 ± 0.002	
$T = 318.15$ K				$T = 318.15$ K			
0.0101	0.99104 ± 0.00001	0.588 ± 0.002		0.0559	0.99396 ± 0.00001	0.602 ± 0.001	
0.0253	0.99188 ± 0.00001	0.593 ± 0.002		0.0712	0.99517 ± 0.00003	0.607 ± 0.001	
0.0406	0.99287 ± 0.00001	0.597 ± 0.003		0.0866	0.99644 ± 0.00002	0.612 ± 0.002	
D-Mannitol + aq. NA							
$T = 298.15$ K				$T = 298.15$ K			
0.0100	0.99808 ± 0.00001	0.896 ± 0.001	1.3329 ± 0.0001	0.0555	1.00152 ± 0.00002	0.918 ± 0.001	1.3354 ± 0.0001
0.0251	0.99912 ± 0.00004	0.903 ± 0.002	1.3338 ± 0.0001	0.0707	1.00283 ± 0.00002	0.926 ± 0.001	1.3362 ± 0.0001
0.0403	1.00028 ± 0.00003	0.910 ± 0.002	1.3346 ± 0.0002	0.0860	1.00423 ± 0.00004	0.934 ± 0.001	1.337 ± 0.0001
$T = 308.15$ K				$T = 308.15$ K			
0.0101	0.99500 ± 0.00003	0.724 ± 0.003		0.0557	0.99824 ± 0.00002	0.744 ± 0.002	
0.0252	0.99596 ± 0.00001	0.730 ± 0.001		0.0710	0.99950 ± 0.00002	0.752 ± 0.001	
0.0404	0.99705 ± 0.00002	0.737 ± 0.001		0.0863	1.00089 ± 0.00003	0.759 ± 0.002	
$T = 318.15$ K				$T = 318.15$ K			
0.0101	0.99107 ± 0.00002	0.589 ± 0.002		0.0559	0.99423 ± 0.00004	0.607 ± 0.001	
0.0253	0.99197 ± 0.00001	0.595 ± 0.001		0.0713	0.99547 ± 0.00002	0.614 ± 0.002	
0.0406	0.99302 ± 0.00001	0.601 ± 0.003		0.0867	0.99686 ± 0.00003	0.620 ± 0.002	
D-Sucrose + aq. NA							
$T = 298.15$ K				$T = 298.15$ K			
0.0100	0.99874 ± 0.00003	0.898 ± 0.001	1.3333 ± 0.0001	0.0558	1.00526 ± 0.00002	0.933 ± 0.002	1.3370 ± 0.0002
0.0252	1.00079 ± 0.00005	0.910 ± 0.001	1.3345 ± 0.0001	0.0712	1.00764 ± 0.00002	0.946 ± 0.002	1.3383 ± 0.0001

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