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Effect of Solvents on the Ultrasonic Velocity and Allied Parameters of Nifedipine Drug in Different Mixed Solvents at 300 K

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ABSTRACT

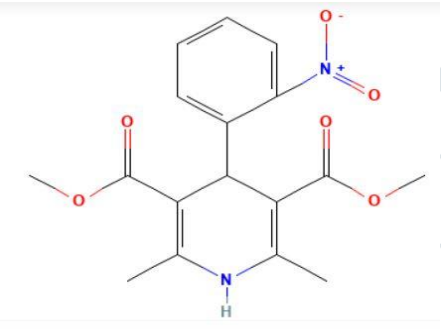
The scientific investigations in the field of ultrasonic velocity measurements in drugs solutions in various binary solvents mixture is carried out. The measurements were performed with ultrasonic interferometer (Mittal Enterprises, New Delhi) at a frequency of 2MHz with a tolerance of ± 0.005%. *The density, viscosity and ultrasonic velocity for Nifedipine drug have been investigated by experimental procedures in order to understand the effect of ion-ion interaction and influence of ions on solvents structure in different medium at 300K in the concentration range of 0.02 to 0.06 mol* dm^{-3}. *In this present work various acoustical parameters such as apparent molar compressibility* (φ_k), *apparent molar volume* (φ_v), *intermolecular free length* (L_f), *adiabatic compressibility* (β_s), *specific acoustic impendence(Z),etc. have been evaluated. Ultrasonic studies provide valuable information in understanding the molecular behavior and intermolecular interactions of Nifedipine drug in different solvent mixtures. The variation of these acoustic parameters is explained in terms of solute-solvent molecular interaction occurring in drug solutions.*

Introduction

Recent developments have found use of ultrasound measurements in medicine, engineering, industry and agriculture[1-2]. Solvation describes the interaction of solvent with dissolved molecules. Both ionized and uncharged molecules interact with solvent, strength and nature of this interaction influence many properties of the solute as well as influencing the properties of the solvent such as viscosity and density. Ion-solvation is the back bone of solution chemistry [1-2]. Ultrasonic waves and related thermodynamic parameters provided valuable information about the structure of solid. The measurement of ultrasonic velocity has been adequately employed in understanding the nature of molecular interactions in pure liquids[3-6] and liquid mixtures[7-8]. Ultrasonic propagation parameters yield valuable information regarding the behavior of liquid systems, because intramolecular and intermolecular association, dipolar interactions, complex formation and related structural changes affect the compressibility of the system which in turn produces corresponding variations in the ultrasonic velocity. The acoustical and thermodynamical parameters obtained in ultrasonic

study show that the ion solvation is accompanied by the destruction or enhancement of the solvent structure[9-12]. Excess thermodynamic properties of liquid mixtures are of great interest to conveniently design industrial processes and also to provide valuable information on the molecular interactions required for optimizing thermodynamic models. When two or more liquids are mixed there occur some changes in physical and thermodynamic properties because of free volume change, change in energy and change in molecular orientations. Derived thermodynamic and acoustical parameters like internal pressure, free volume and acoustic impedance are of considerable interest in understanding the intermolecular orientations in binary liquid mixtures[13-14]. Excess thermodynamic properties of mixtures are useful in the study of molecular orientations and arrangements[15-16].

For the present study Nifedipine drug is selected and its chemical structure is



Dimethyl 2, 6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

The Nifedipine inhibits the entry of calcium ion by blocking these voltage-dependent L-type calcium channels in vascular smooth muscle and myocardial cells. It works by affecting the movement of calcium into the cells of the heart and blood vessels. As a result, Nifedipine drug relax blood vessels and increases the supply of blood and oxygen to the heart while reducing its workload. So, it was found important to study ultrasonic and thermodynamic behavior of the dugs which may lead to some new findings. The acoustic properties of Nifedipine drug have been studied in 40% Ethanol-water, 40% Acetone-water and 40% DMF-water solutions at 300K.

Experimental

Ultrasonic velocity measurements were made by using an ultrasonic interferometer (Mittal Enterprises, New Delhi) at a frequency of 2MHz with a tolerance of ± 0.005%. All the measurements were carried out at 300K.The temperature was maintained constant by circulating water from controlled water bath (accuracy ± 0.1^0C). For the present work ethanol, acetone and dimethyl formamide solvents used which are of AR grade and were purified by the usual procedure. Densities, viscosities and ultrasonic velocities were measured at 300K over a wide range of composition. Densities were determined by using 25ml capacity gravity bottle and digital balance with an accuracy of 0.0001g. The viscosities were measured by precalibrated Ostwald viscometer.

Theory

Various Acoustic parameters such as apparent molar compressibility (φ_k), apparent molar volume (φ_v), adiabatic compressibility (β_s), specific acoustic impendence (Z), intermolecular free length (L_f), Limiting apparent molar volume (φ^0_v), Limiting apparent molar compressibility (φ^0_k) were determined using following relations.

1. Ultrasonic velocity $u = \lambda\upsilon$
   Where υ is the frequency of ultrasonic waves and λ is the measured wavelength of ultrasonic waves in solution.
2. Adiabatic compressibility (Newton-Laplace equation) $\beta_s = 1/ u^2_s \rho_s$
3. Apparent molar volume $\varphi_v = 10^3(\rho_0-\rho_s)/m-\rho_0 \rho_s + M/\rho_0$
4. Apparent molar compressibility $\varphi_k = 10^3(\rho_0\beta_s-\rho_s\beta_0)/m-\rho_s \rho_0 + \beta_s M/\rho_s$
5. Limiting apparent molar volume $\varphi_v=\varphi^0_v + S_v C^{1/2}$
6. Limiting apparent molar compressibility $\varphi_k=\varphi^0_k + S_k^{1/2}$
7. Intermolecular free length $L_f = K (\beta_s)^{1/2}$
8. Specific acoustic impendence $Z = \rho.u$

TableNo.1

Experimental Data of Density, Ultrasonic Velocity and Viscosity of Nifedipine Drug in Different Solvents at 300 K

Solvents	Conc.mol.dm^{-3}	Density ρ_sKgm^{-3}	Ultrasonic Velocity(u)m/s	Viscosityx10^{-3} Nsm^{-2}
40% Ethanol-Water Medium	0.02	928. 07	1543.7	1.1625
	0.03	928.28	1554.0	1.1632
	0.04	928.65	1576.7	1.1643
	0.05	928.79	1588.3	1.1655
	0.06	928.86	1595.9	1.1687
40% Acetone-Water Medium	0.02	1054.44	1649.3	1.2335
	0.03	1054.56	1661.2	1.2369
	0.04	1054.61	1675.6	1.2385
	0.05	1054.72	1681.9	1.2395
	0.06	1054.95	1689.7	1.2399
40% DMF-Water Medium	0.02	1012.41	1543.3	1.0531
	0.03	1012.52	1567.5	1.0543
	0.04	1012.73	1571.6	1.0556
	0.05	1012.84	1582.5	1.0567
	0.06	1012.96	1599.8	1.0586

Table no.2

Variation of some acoustical parameters with concentration of Nifedipine Drug in different Solvents at 300K

Solvents	Conc.mol.dm^{-3}	β_s x 10^{-10} Pa^{-1}	Φ_v x10^{10} m^{3}mol^{-1}	Φ_k x10^8 m^{3}mol^{-1} Pa^{-1}	L_f X 10^{-11} (m)	Z x 10^5 Kg m^{-2} sec^{-1}
40% Ethanol - Water Medium	0.02	4.2611	4.96536	-50.8002	1.2448	15.2023
	0.03	4.2026	3.31020	-78.6983	1.2362	15.3109
	0.04	4.0805	2.48263	-103.195	1.2181	15.5431
	0.05	4.0181	1.98608	-121.5451	1.2087	15.6673
	0.06	3.9789	1.655051	-133.3359	1.2028	15.7483
40% Acetone-Water Medium	0.02	3.7330	4.96536	-199.967	1.1651	16.2423
	0.03	3.6782	3.310208	-216.0368	1.1565	16.3661
	0.04	3.6135	2.48263	-235.350	1.1463	16.5170
	0.05	3.5842	1.986085	-244.2635	1.1416	16.5885
	0.06	3.5494	1.65505	-254.877	1.1360	16.6739
40% DMF-Water Medium	0.02	4.2168	4.96536	-98.2474	1.2383	15.2821
	0.03	4.1794	3.31020	-8301099	1.2328	15.3533
	0.04	4.1705	2.48261	-77.7607	1.2314	15.3745
	0.05	4.1433	1.98608	-70.523	1.2274	15.4286
	0.06	4.1029	1.65505	-55.899	1.2214	15.5085

Table-3

Limiting values of ϕ^0_v and ϕ^0_k along with slope (S_v & S_k) for Nifedipine Drug in different medium at 300K temperature

Temp. T (K)	Medium	Parameters			
		ϕ^0_v x 10^{-5} m^{3}mol^{-1}	ϕ^0_k x 10^{-14} m^{3}mol^{-1}pa^{-1}	S_vx 10^{-5} m^{3}mol$^{-3/2}$dm$^{3/2}$	S_k x 10^{-14} m^{3}mol$^{-3/2}$dm$^{3/2}$pa^{-1}
300K	40% Ethanol -H_2O	-148.634	-77.65	473.88	326.95
	40% Acetone- H_2O	-76.643	-256.17	448.771	409.523
	40% DMF- H_2O	4.854	545.26	61.342	-1483.37

Table-4

A and β, coefficient values at 300 K in different medium for Nifedipine Drug

Medium	Coefficient	300K
40% Ethanol-Water medium	A	1.564
	β	-0.253
40% Acetone-Water medium	A	1.852
	β	-0.384
40% DMF-Water medium	A	0.453
	β	-0.118

Results and discussion:

Table 1 shows that density (ρ), ultrasonic velocity (u) and viscosity (η) increases with increase in concentration for all three systems. The increase in ultrasonic velocity is due to decrease in intermolecular free length (L_f) as shown in table 2. This suggests that there is a strong interaction between Nifedipine drug and solvent molecule. Adiabatic compressibility (β_s) is a measure of intermolecular association or repulsion calculated from the measured ultrasonic velocity (u) and density (ρ). Adiabatic compressibility is found to decrease with increase in concentration. Since adiabatic compressibility is inversely related to the product of density and ultrasonic velocity based on this the compressibility is expected to decrease which has observed in the present case. When the sound waves travel through the solution, certain part of it travels through the medium and rest gets reflected by the ion i.e. restriction for flow of sound velocity by the ions. The character that determines the restriction movement of sound waves is known as acoustic impendence (Z). It has been found that acoustic impendence increases with increase in concentration. The apparent molar compressibility (φ_k) explains the solute-solvent and solute- solute interactions in solution and was calculated by using the equation no. (iv). The apparent molar volume (φ_v) is defined as the change in volume of solution for the added one mole of a particular component at constant temperature and pressure. It is thermodynamic property which helps in elucidating solvation behavior of electrolyte in solution. Apparent molar volume was evaluated from the density of solution and solvent.

It is evident from the table 3 that φ^0_k values are negative for 40% EtOH-water and 40% Acetone-water but for 40%DMF-water φ^0_k values are positive. The negative φ^0_k values are suggest solute- solvent interaction whereas positive values are due to solute- solute interaction, is further confirmed by φ^0_v values which are positive for 40% DMF-water and negative for 40%EtOH-water and 40% Acetone-water of the drug. Sv is a measure of solute – solvent interaction. It is observed from the table 3 that Sv values are higher in 40% EtOH-water and 40% Acetone-water and low in 40% DMF-water solution. This confirms that in 40% DMF-water solution solute- solute interactions and in 40% EtOH-water and 40% Acetone-water solute – solvent interaction predominates.

The viscosity β -Co-efficient has been derived from Jones-Dole equation

$$(c> 0.1m)\ \eta_r\text{-}1 / C^{1/2} = A+B\ C^{1/2}$$

Where $\frac{\eta}{\eta 0} = \eta_r$ is the relative viscosity A and β are the characteristics of the solute and solvent. A is Falkenhagen coefficient represent the contributor from solute-solute interaction and β is Jones Dole coefficient known to depend on the size of the solute particle and on the interaction between solute and solvent.

They were obtained by a least – squares treatment as intercept and slope of the linear plot of ηr-1 / $C^{1/2}$ Vs $C^{1/2}$. The graph for each system given linear straight-line showing validity of Jones-Dole equation. The slope of straight line gives value of β- co-efficient.

The viscosity A coefficient represent the ion-ion interactions and negative values have shown some physical significance. However negative 'A' values have also been reported to be in other solvents in some studies. The large and small value of 'A' shows the stronger and weaker solute – solute interactions respectively.

When solute is introduced into solvent of organic-water mixture it will interfere with the ordered structure of water in the solute's co-sphere. As only one solute is present so such variation in the values of A can be explained.

In the present study viscosity of liquid solutions increases with increase in concentration of Nifedipine drugs solution in 40% ethanol-water, 40% acetone-water and 40% DMF-water mixture. The increase in viscosity with increase in concentration may be attributed to the increase in solute solvent interactions.

Viscosity β-coefficients have been established from ion- solvent interactions and are responsible for introducing order or disorder in the structure of the solvent. Solute with negative β-Coefficient is characterized as structure breakers indicating weak solute-solvent interactions. [18-23]

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