

Research Paper

Chemistry

Study of molecular interactions of Chlorpromazine hydrochloride in different solvents at 308.15K.

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ABSTRACT The measurements of density, viscosity and speed of sound of chlorpromazine hydrochloride have been determined by experimental procedures using bicapillary pyknometer, Ostwald viscometer and ultrasonic interferometer respectively. From the experimental data various acoustical parameters such as apparent molar compressibility (fk), apparent

molar volume (fv), adiabatic compressibility (β s), specific acoustic impendence (Z), intermolecular free length (Lf) have been evaluated. The concentration range is 0.02 to 0.1 mol dm-3

The measurements are conducted at 308.15K in different solvents. The results are interpreted in terms of molecular interactions occurring in these

KEYWORDS:

Introduction

Ultrasonic and living beings were in co-existence from the prehistoric days. The use of ultrasound was proved to be useful probe for generating more information on many areas and review articles on various topics. Ultrasonic waves provide valuable information about the molecular interaction in pure liquids¹, aqueous solutions², liquid mixtures³ and also provide valuable information about the structure of solids ⁴.

For the present study drug Chlorpromazine hydrochloride is selected. This drug is used as antipsychotic, neuroleptic and psychosedative. The acoustic properties of Chlorpromazine hydrochloride have been studied in 20% Methanol-water, 20% Dioxane-water and 20% DMF-water solutions at 308.15 K.

Experimental

Solvents methanol, dioxane and dimethyl formamide used in the present work were of AR grade and were purified and dried by the usual procedure. Densities, viscosities and ultrasonic velocities were measured at 303 K over a wide range of composition. Densities were determined by using bicapillary pyknometer. The viscosities were measured by precalibrated Ostwald type viscometer with an accuracy of about \pm 0.1K. Ultrasonic velocity measurements were made by using an ultrasonic interferometer (Mittal Enterprises, New Delhi) at a frequency of 2MHz with a tolerance of \pm 0.005%. All the measurements were carried out at 308.15 K.

Theory

Acoustic parameters such as apparent molar compressibility (fk), apparent molar volume (fv), adiabatic compressibility (β s), specific acoustic impendence (Z), intermolecular free length (Lf), Limiting apparent molar volume (f0v), Limiting apparent molar compressibility (f0k) were determined using following relations. Ultrasonic velocity

λυ	1
Adiabatic compressibility	β
1/u ² , p,	2
Apparent molar volume	
$\phi_v = 10^3 (\rho_0 \cdot \rho_s) m \cdot \rho_0 \rho_s + M (\rho_0 \dots$	3
Apparent molar compressibility	φ _k
$10^{3}(\rho_{0}\beta_{s}-\rho_{s}\beta_{0})/m-\rho_{s}\rho_{0}+\beta_{4}M/\rho_{s}$	- 4
Intermolecular free length	Lf
$\equiv K (\beta_i)^{1/2}$	5
Specific acoustic impendence	Z
= p.u 6	
Limiting apparent molar volume	Φ.,
$= \phi_{v}^{0} + S_{v}C^{1/2}7$	
Limiting apparent molar compress	ibility ϕ_k
$= \phi_k^0 + S_k^{1/2}$ 8	

Table no.1 Experimental Data of Density, Ultrasonic Velocity and Viscosity of CPZ in different solvent at 308.15 K

Solvents	Conc.mol.dm ⁻³	Density p _s Kgm⁻³	Ultrasonic Velocity(u) m/s	Viscosity x10 ⁻³ Nsm ⁻²
	0.02	1032.09	1579.5	1.02187
ater	0.04	1032.16	1583.0	1.02817
H-Wa	0.06	1032.66	1586.2	1.03248
MeO	0.08	1032.94	1590.1	1.03855
20% Med	0.1	1033.15	1594.1	1.04601
	0.02	1032.09	1579.5	1.17061
Nater	0.04	1032.16	1583.0	1.17526
ane-\	0.06	1032.66	1586.2	1.18346
Diox	0.08	1032.94	1590.1	1.18835
20% Med	0.1	1033.15	1594.1	1.19470
	0.02	990.19	1478.3	0.84832
er	0.04	990.91	1480.4	0.85378
-Wat	0.06	991.95	1482.1	0.85832
DMF	0.08	993.19	1484.3	0.86425
20% Meo	0.1	993.95	1485.6	0.86855

Table no.2 Variation of some acoustical parameters with concentration of

CPZ in different solvents at 308.15 K

Solvents	Conc.mol.dm ⁻³	$\beta_{s_1 \times 10}$ -10	ው x10 ⁻⁵ m ⁵ mol ⁻¹	Ф ₅ х10 ⁻¹⁴ m ¹ mol ⁻¹ Ра ⁻¹	L,10 ⁻¹¹ (m)	Z x 10 ⁵ Kg m ⁻² sec ⁻¹
-Water	0.02	4.2188	-85.87	-50.943	4.1079	15.3968
1eOH	0.04	4.2112	-27.12	-20.731	4.1042	15.4167
~	0.06	4.2023	-6.51	-10.458	4.0999	15.4341
ш	0.08	4.1898	3.30	-6.0120	4.0937	15.4613
20% Medi	0.1	4.1800	9.19	-3.0787	4.0889	15.4830

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xane- im	0.02	3.9039	-52.0	-72.8134	3.9516	16.2595
idiu	0.04	3.8878	-8.39	-33.7004	4.1000	16.2936
Ň	0.06	3.8736	4.72	-20.6503	4.0926	16.3273
ater	0.08	3.8555	11.8	-14.5436	4.0830	16.3679
20 Wã	0.1	3.8295	16.1	-11.6627	4.0692	16.4250
Water	0.02	4.6212	9.85	372.723	4.4700	14.6379
4F.	0.04	46047	21.0	189.584	4.4621	14.6694
	0.06	4.5893	24.2	128.426	4.4546	14.7016
diur	0.08	4.5700	25.5	97.1877	4.4452	14.7419
20% Me	0.1	4.5586	26.7	79.4595	4.4397	14.7661

Table-3- Limiting values of ϕv and ϕk along with slope (Sv & Sk) for CPZ

in different medium at 308.15 K temperature

		Parameters			
Temp. T (K)	Medium	φ ⁰ × 10 ⁻⁵ m³mol ⁻¹	φ ⁰ × 10 ⁻¹⁴ m ³ mol ⁻¹ pa ⁻¹	S x 10 ⁻⁵ m ³ mol ⁻ ³/2dm ^{3/2}	S _, x 10 ⁻¹⁴ m ³ mol ⁻ ^{3/2} dm ^{3/2} pa ⁻¹
	20%M-W	-147.1	-81.33	530.4	266.1
308.15 K	20%D-W	-95.22	-111.5	341.8	341.2
	20%DMF-W	6.760	601.2	66.31	-1753.0

Table-4 A and β, coefficient values at at 308.15 K in different medium for CPZ

Medium	coefficient	Temp 308.15 K
200/ Mathanal Water medium	A	0.9500
20%Methanoi-water medium	β	-0.101
20% Dioyana Water medium	A	1.527
	β	-0.174
20% DME Water medium	A	0.453
	β	-0.039

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 (Lf) as shown in table 2. This suggests that there is a strong interaction between chlorpromazine and solvent molecule. Adiabatic compressibility (Bs) is a measure of intermolecular association or repulsion calculated from the measured ultrasonic velocity (u) and density (p). Adiabatic compressibility is found to decrease with increase in concentration5. 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 travels through the solution, certain part of it travels through the medium and rest gets reflected by the ion6 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 (fk) explains the solute-solvent and solute- solute interactions in solution and was calculated by using the equation no. 4. The apparent molar volume (fv) 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 f0k values are negative for 20% MeOH-water and 20% Dioxane-water but for 20%DMF-water f0k values are positive. The negative f0k values are suggest solute- solvent interaction whereas positive values are due to solute- solute interaction, is further confirmed by f0v values which are positive for 20% DMF-water and negative for 20% MeOH-water and 20% Dioxane-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 20% MeOH-water and 20% Dioxane-water and low in 20% DMF-water solution. This confirms that in 20% DMF-water solution solute- solute interactions and in20% MeOH-water and 20% Dioxane-water solute - solvent interaction predominate.

The viscosity B-Co-efficient has been derived from Jones-Dole equation27

 $(c>0.1m)\eta_r-1~/~C^{1/2}=A+B~C_{1/2}~~Where~~\eta r~~is~the~relative~viscosity.~A~~and~B~~are~the~characteristics~of~the~solute$ and solvent. A is Falkenhagen coefficient represent the contributor from solute-solute interaction and B 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 $\,\eta,-1$ / $C^{1/2}\,Vs$ $C^{1/2}$ The graph for each system given linear straight line showing validity of Jones-Dole equation. The slope of straight line gives value of B 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.7-9

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 solutes 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 antipsychotic drugs salts solution in 20% methanol -water, 20% dioxane-water and 20% DMF-water mixture. The increase in viscosity with increase in concentration may be attributed to the increase in solute solvent interactions.

Viscosity B coefficients have been established to arise from ion- solvent interactions and are responsible for introducing order or disorder in the structure of the solvent. Solute with negative B Coefficient is characterized as structure breakers indicating weak solute-solvent interactions. Such type of results is also shown by Eyring et al.¹⁰



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