Ultra Chemistry Vol. 8(3), 437-441 (2012).

Ultrasonic Studies of molecular interactions in different solvents of 4-Methylumbelliferyl- β -D-glucuronide (4-MUG) at 303K.

B. JAGAN MOHAN REEDY[a], R. ANJIBABU[a], RAVI JUMLE[b] and USHA WASNIK[c]

[a]Department of Chemistry, Adikavi Nannaya University, Rajahmundyr, AP-533105 (INDIA)
[b]Department of Chemistry, Shivaji Science College, Akot Dist : Akola (M.S.) (INDIA)
[c]Department of Chemistry, Arts Science and Commerce College, Chikhaldara Dist, Amravati (M.S.) 444807 (INDIA)

(Acceptance Date 1st November, 2012)

Abstract

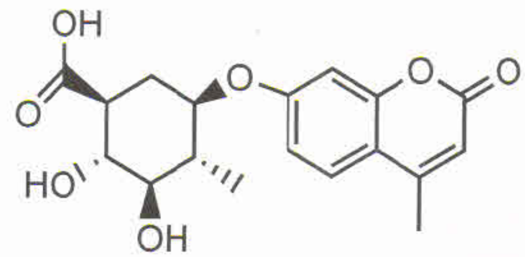
The measurements of density, viscosity and speed of sound of 4-Methylumbelliferyl-β-D-glucuronide have been determined by experimental procedures using bicapillary pyknometer, Ostwald viscometer and ultrasonic interferometer respectively. From the experimental data various acoustical parameters such as apparent molar compressibility (ϕ_k), apparent molar volume (ϕ_v), adiabatic compressibility (β_s), specific acoustic impendence (Z), intermolecular free length (L_f) have been evaluated. The concentration range is 0.02 to 0.1 mol dm^{-3}

The measurements are conducted at 303K in different solvents. The results are interpreted in terms of molecular interactions occurring in these solutions.

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 liquids[1], aqueous solutions[2], and liquid mixtures[3] and also provide valuable information about the structure of solids[4].

For the present study 4-Methylumbelliferyl-β-D-glucuronide is selected, which was synthesized by Lopez-Lopez *et.al.* protocal[5]. 4 -Methyl umbelliferyl-β-D-glucuronide is a fluorogenic substance, which is widely used for the detection of Escherichia Coli in water[6-8], food and other products for human consumption through its ability to detect activity of b-d-glucuronidase (GUR).



MUG

This molecule is used as antipsychotic, neuroleptic and psychosedative. The acoustic properties of 4-Methylumbelliferyl-B-D-glucuronidehydratehave been studied in 30% Methanol-water, 30% Dioxane-water and 30% DMF-water solutions at 303 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 Oswald type viscometer with an accuracy of about ± 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 ± 0.005%. All the measurements were carried out at 303 K.

Theory :

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.

Ultrasonic velocity $u = \lambda\upsilon$ --- (1)

Adiabatic compressibility $\beta_s = 1/u^2_s \rho_s$--- (2)

Apparent molar volume $\phi_v = 10^3(\rho_0-\rho_s)/m\text{-}\rho_0 \rho_s + M/\rho_0$ --- (3)

Apparent molar compressibility

$\phi_k = 10^3(\rho_0\beta_s-\rho_s\beta_0)/m\text{-}\rho_s \rho_0+\beta_s M/\rho_s$ --- (4)

Intermolecular free length $L_f=K(\beta_s)^{1/2}$ --- (5)

Specific acoustic impendence $Z=\rho.u$ --- (6)

Limiting apparent molar volume $\phi_v=\phi^0_v+S_vC^{1/2}$ —(7)

Limiting apparent molar compressibility

$\phi_k = \phi^0_k + S_k^{1/2}$--- (8)

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 chlorpromazine 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[5]. 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 ion[9]

Table 1. Experimental Data of Density, Ultrasonic Velocity and Viscosity of 4-Methylumbelliferyl- β -D-glucuronide in different solvent at 303K

Solvents	Conc.mol. dm^{-3}	Density ρ_s Kgm^{-3}	Ultrasonic Velocity(u)m/s	Viscosity $x10^{-3} Nsm^{-2}$
30% MeOH-Water Medium	0.02	1031.09	1580.5	1.02186
	0.04	1031.16	1584.0	1.02956
	0.06	1031.66	1587.2	1.03685
	0.08	1031.94	1591.1	1.03915
	0.1	1032.15	1595.1	1.04332
30% Dioxane-Water Medium	0.02	1033.10	1581.5	1.17158
	0.04	1033.17	1583.2	1.17658
	0.06	1033.65	1587.2	1.18389
	0.08	1033.98	1591.3	1.18912
	0.1	1034.23	1534.1	1.19521
30% DMF-Water Medium	0.02	991.19	1481.3	0.84932
	0.04	991.93	1483.4	0.85236
	0.06	992.56	1483.9	0.85925
	0.08	993.16	1485.6	0.86425
	0.1	994.09	1487.02	0.86955

Table 2. Variation of some acoustical parameters with concentration of 4-Methylumbelliferyl- β -D-glucuronide in different solvents at 303 K

Solvents	Conc.mol. dm^{-3}	β_s $x10^{-10}$ Pa^{-1}	$\Phi_v x10^{-5}$ m^3mol^{-1}	Φ_k $x10^{-14}$ $m^3mol^{-1}Pa^{-1}$	$L_{f}x10^{-11}$ (m)	Z x 10^5Kg $m^{-2}sec^{-1}$
30% MeOH-Water Medium	0.02	4.2248	-85.9812	-51.001	4.1101	15.3897
	0.04	4.2196	-28.75	-20.854	4.1023	15.4254
	0.06	4.2096	-6.85	-10.532	4.0986	15.4456
	0.08	4.1986	3.41	-6.0213	4.0925	15.4702
	0.1	4.1826	9.39	-3.0869	4.0888	15.4963
30% Dioxane-Water Medium	0.02	3.9039	-52.0	-72.8134	3.9516	16.2595
	0.04	3.8878	-8.39	-33.7004	4.1000	16.2936
	0.06	3.8736	4.72	-20.6503	4.0926	16.3273
	0.08	3.8555	11.8	-14.5436	4.0830	16.3679
	0.1	3.8295	16.1	-11.6627	4.0692	16.4250
30% DMF-Water Medium	0.02	4.6212	9.85	372.723	4.4700	14.6379
	0.04	46047	21.0	189.584	4.4621	14.6694
	0.06	4.5893	24.2	128.426	4.4546	14.7016
	0.08	4.5700	25.5	97.1877	4.4452	14.7419
	0.1	4.5586	26.7	79.4595	4.4397	14.7661

Table 3. Limiting values of ϕ_v and ϕ_k along with slope (S_v & S_k) for 4-Methylumbelliferyl-β-D-glucuronide in different medium at 303K temperature

Temp. T (K)	Medium	Parameters			
		$\phi^0_v \times 10^{-5}$ m^3mol^{-1}	$\phi^0_k \times 10^{-14}$ $m^3mol^{-1}pa^{-1}$	$S_v \times 10^{-5}$ $m^3mol^{-3/2}dm^{3/2}$	$S_k \times 10^{-14} m^3$ $mol^{-3/2}dm^{3/2}pa^{-1}$
303K	30%M-W	-147.1	-81.33	530.4	266.1
	30%D-W	-95.22	-111.5	341.8	341.2
	30%DMF-W	6.760	601.2	66.31	-1753.0

Table 4. A and β, coefficient values at at 303K in different medium for 4-Methylumbelliferyl-β-D-glucuronide

Medium	coefficient	Temp 303.15 K
30%Methanol- Water medium	A	0.9500
	β	-0.101
30%Dioxane- Water medium	A	1.527
	β	-0.174
30% DMF- Water medium	A	0.453
	β	-0.039

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. 4.

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[10].

It is evident from the table 3 that ϕ^0_k values are negative for 30% MeOH-water and 30% Dioxane-water but for 30% 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 30% DMF-water and negative for 30% MeOH-water and 30% Dioxane-water of the drug. S_v is a measure of solute – solvent interaction. It is observed from the table 3 that Sv values are higher in 30% MeOH-water and 30% Dioxane-water and low in 30% DMF-water solution. This confirms that in 30% DMF-water solution solute- solute interactions and in30% MeOH-water and 30% Dioxane-water solute – solvent interaction predominate.

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