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Thermo acoustical studies of molecular interaction of N-[[(2S)-1-ethylpyrrolidin-2-yl] methyl]-2-methoxy-5-sulfamoylbenzamide at different temperature.

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ABSTRACT

Density(ρ),Viscosity(η) and Ultrasonic Velocity (U) of an alcoholic solution of N-[[(2S)-1- ethylpyrrolidin-2-yl]methyl]-2-methoxy-5-sulfamoylbenzamid drug(NSB) 2.5mM,5.0mM and 10mM were measured at 300, 305 and 310K. The resulting data were used to calculate various acoustical parameters ,acoustic impedance (Z), adiabatic compressibility(β), Intermolecular free length (L_f), Wada's Constant (W), Rao's Constant (R), free volume (V_f) , were calculated which provides valuable information regarding drug-alcohol interaction

Keywords NSB, Acoustical parameters, Inter molecular interaction, drug-alcohol interaction.

INTRODUCTION

Ultrasound refers to such high frequency sound waves that they can't be heard. Now a day's Ultra-Sonic technology due to non-destructive nature [1–3], is used in a variety of applications in medicine, biology, industry, materials science agriculture, oceanography, sonochemistry etc. Ultra-sound waves have been used extensively as chemical additives for order to improve the production yield of produced foods, and also useful in the preparation of biomaterials, protein microspheres, polymer and polymer surface modifications, etc. for material chemistry [4-7].

Ultrasounds provide the most exciting field of science research among scientists since they provide useful information concerning molecular structure (MO), molecular order, molecular packaging, inter- and internal molecular interactions [8] etc. In the ultrasound and other related thermoacoustic parameters The literary survey reveals that a significant number of researchers researched ultrasonic molecular interactions and viscosity measurement [9-10].

N-[[(2S)-1-ethylpyrrolidin-2-yl]methyl]-2-methoxy-5-sulfamoylbenzamide.It is a substituted benzamide antipsychotic. It is also said to have properties that boost mood. Mainly used for the treatment of reflexion, indigestion, persistent cardiovascular syndrome, bowel syndrome and dyspepsia.

METHODOLOGY

The solutions of different concentration (mM) of N-[[(2S)-1-ethylpyrrolidin-2-yl]methyl]-2-methoxy-5-sulfamoylbenzamide (Molar mass = 341.4g/mole) were prepared in alcohol as the solvent. The densities (ρ) of these binary solutions were measured accurately using 25 ml specific gravity bottle in an electronic balance with an accuracy of ±0.0001g. The basic parameter ultrasonic velocity (U) had been measured on Digital Ultrasonic Pulse Echo Velocity Meter (Vi Microsystems Pvt. Ltd. Model VCT-70 with single frequency of 2 MHz having an accuracy of 0.1%. The viscosities (η) of solutions were determined by using Ostwald's viscometer by calibrating with doubly distilled alcohol with an accuracy of ±0.001 Pa.sec. Surface tension was measured by using Stalagmometer. The basic parameter U, η and ρ of various concentrations of drug viz.,2.5, 5, 10mM were measured at 300, 305 and 310K. Thermostatically controlled alcohol circulation system is used to maintain the temperature with an accuracy of 0.05 0C. For all solutions and pure components, triplicate measurements were performed. The various acoustical parameters were calculated from U, η and ρ values by using standard formulae as shown below-

Molecular Formula $C_{15}H_{23}N_3O_4S$

The various acoustical parameters such as adiabatic compressibility (β), intermolecular free length (L_f), relaxation time (τ), free volume (V_f), internal pressure (Πi), acoustic impedance (Z), attenuation (α/f^2), Rao's constant (R), molar volume (V_m),cohesive energy (CE) were calculated by applying the known expressions [11].

1. **Adiabatic compressibility (β):**

$$\beta = \frac{1}{U^2\rho} \quad Kg^{-1}ms^2$$

U= velocity; ρ= Density of liquid

2. **Specific Acoustic impedance (Z):**

$$Z = U^*\rho \quad Kg^{-1}ms^{-2}s^{-1}$$

U= velocity; ρ= Density of solution

3. **Internal Pressure (πi):**

$$\pi_i = b\,R\,T\,[K\eta/U]^{1/2}\left[\frac{\rho^{2/3}}{M^{7/6}}\right] \quad Nm^{-2}$$

Where, K = Independent constant (4.28 x 10^9);
T =Absolute temperature,
η = Viscosity in NSm^{-2};
U = Ultrasonic velocity in ms^{-1}
ρ = Density in $kgm^{-3}$of the liquid;
b= 2 for all liquid,
R=Gas Constant (8.314 J / mol. K)

4. **Absorption coefficient or Attenuation (α/f^2) :**

$$\alpha = 8\pi i^2\,\eta f^2/3\rho U^3 \quad NPm^{-1}s^2$$

Where f is the frequency of ultrasonic wave

5. **Molar compressibility or Wada's constant (W) :**

$$W = [M.\beta^{1/7}]/\rho$$

Where
ρ =density, M=Molecular weight,
β = adiabatic compressibility
.

6. **Rao's constant or molar sound velocity (R) :**

$$R = M/\rho[U]^{1/2}$$

Where,
M = Molecular Weight,
ρ = density
U = Ultrasonic Velocity

7. **Free volume (Vf) :**

$$V_f = [M_{eff}\,U/K\eta]^{1/2} \quad m^3$$

Where
M_{eff} = effective molecular weight,

K is a temperature independent constant (4.28 x10^9 for all liquid)

8. Relaxation time (τ):

τ = 4/3ηk_2 second

Where,

η=Viscosity of solution

k_2 =1/$U^2\rho$ is the isentropic compressibility of liquid

9. Molar Cohesive Energy(Binding Force)(CE):

CE= πi xVm KJ/Mole

Where,

πi =Internal Pressure,

Vm =Molar Volume

10. Intermolecular Free Length(L_f):

L_f=KT x $\beta^{1/2}$

Where, KT = The Temperature dependent constant known as Jacobson's Constant

KT = (93.875 + 0.375 x T),

T=Absolute Temp. in Kelvin.

11. Molar Volume:

Vm= ρ/M

Where,

ρ= density of solution,

M=Molecular weight

RESULTS AND DISCUSSION

Measured parameters such as ultrasonic velocity, density and related thermo-acoustical parameters like adiabatic compressibility (β), intermolecular free length (L_f), relaxation time (Ʈ), free volume (V_f), internal pressure (Πi), acoustic impedance (Z), Wada's constant (W), ultrasonic attenuation (α/f^2), Rao's constant (R), molar volume (V_m),cohesive energy (CE) of NSB with alcohol at 300K, 305K, and 310K temperatures in different molar concentrations are shown in Table 1a,1b,1c and Table 2a,2b,2c.

There are significant changes in the ultrasonic speed and acoustic impedance when molar concentration is increased. This suggests that hydrogen bonding can lead to complex growth and intermolecular weak association.

Table 1(a) Solution of NSB drug in alcohol at 300 K.

Concentration (mM)	Density (Kgm^{-3})	Viscosity x10^{-3} (Nsm^{-2})	Ultrasonic Velocity (m/s)	Adiabatic compressibility x10^{-10} (m^2 /N)	Intermolecular free length x10^{-11}(m)	Free Volume x10^{-6} (m^3 mol-1)	Rao's constant
2.5mM	977.42	0.9024	1515	3.412	4.11957	111.911	5.9525
5mM	988.86	0.9303	1518	3.394	4.11096	106.451	5.9465
10mM	990.1	0.9592	1524	3.355	4.09225	101.653	5.9471

Table 1(b) Solution of NSB in alcohol at 305K.

Concentration (mM)	Density (Kgm-3)	Viscosity x10^{-3} (Nsm^{-2})	Ultrasonic Velocity (m/s)	Adiabatic compressibility x10-^{10} (m^2 /N)	Intermolecular free length x10-11(m)	Free Volume x10^{-6} (m^3 mol^{-1})	Rao's constant
2.5mM	988.36	0.7549	1525	4.438	4.12557	4.0202	7.005
5mM	990	0.7943	1530	4.402	4.1906	3.7432	7.002
10mM	990.6	0.8139	1538	4.354	4.1675	3.637	7.009

Table 1(c) Solution of NSBin alcohol at 310 K.

Concentration (mM)	Density (Kgm^{-3})	Viscosity x10^{-3} (Nsm^{-2})	Ultrasonic Velocity (m/s)	Adiabatic compressibility x10^{-10} (m^2 /N)	Intermolecular free length x10^{-11}(m)	Free Volume x10^{-6} (m3 mol^{-1})	Rao's constant
2.5mM	990.4	0.7595	1521	5.668	5.2270	148.21	5.002
5mM	992.96	0.7963	1524	5.639	5.2582	136.45	4.99
10mM	993.76	0.8241	1532	5.589	5.2341	129.34	4.996

Table 2(a) Solution of NSB in alcohol at 300 K.

Concentration (mM)	Internal pressure x10^3 (Nm^{-2})	Acoustic Impedance x10^3 (Kg^{-1} m^2 S^{-1})	Molar volume x10^{-3} (m^3/mol)	Wada's constant x10^1	Ultrasonic attenuation x10^{-15} (s^2m^{-1})	Cohesive energy x10^3 (KJ/Mole)	Relaxation time x10^{-6} (S)
2.5mM	17.457	1.623	528.4	1.1139	5.894	8.6251	3.0476
5mM	17.746	1.627	527.7	1.113	6.069	8.7629	3.1442
10mM	18.015	1.635	527.1	1.1133	6.202	8.8919	3.2579

Table 2(b) Solution of NSB in alcohol at 305K.

Concentration (mM)	Internal pressure x10^3 (Nm^{-2})	Acoustic Impedance x10^3 (Kg^{-1} m^2 S^{-1})	Molar volume x10-3 (m3/mol)	Wada's constant x10^1	Ultrasonic attenuation x10^{-15} (s^2m-1)	Cohesive energy x10^3 (KJ/Mole)	Relaxation time x10^{-6} (S))
2.5mM	4.8289	1.504	534.9	1.1339	6.652	2.9775	3.4229
5mM	4.9455	1.512	534.1	1.1334	6.886	3.0345	3.5615
10mM	4.9207	1.521	533.8	1.1345	6.937	3.0625	3.6483

Table 2(c). Solution of NSB in alcohol at 310K

Concentration (mM)	Internal pressure x10^3 (Nm^{-2})	Acoustic Impedance x10^3 (Kg^{-1} m^2 S^{-1})	Molar volume x10^{-3} (m^3/mol)	Wada's constant x10^1	Ultrasonic attenuation x10^{-15} (s^2m-1)	Cohesive energy x10^3 (KJ/Mole)	Relaxation time x10^{-6} (S
2.5mM	16.769	2.335	544.5	1.369	6.075	9.2102	2.1392
5mM	17.2042	2.342	543.1	1.367	6.317	9.4391	2.2623
10mM	17.4869	2.351	542.7	1.368	6.441	9.5767	2.3697

Ultrasonic velocity and adiabatic compressibility have the opposite trend, suggesting the combination of interacting NSB drug and alcohol molecules. The molar concentrations can cause complex formation between component molecules. Adiabatic compression (β) shows an opposite performance in comparison with ultrasonic velocity. Diminishing adiabatic compressibility with rising NSB concentration.The decline in compressibility indicates an increased molecular interaction with a greater conc entration of solvents. The nonlinear density pattern with concentration shows the building and breaking property of compounds due to the forming and weakening of H-bonds. The free length varies not linear, and the molar concentration increases. It indicates a strong interaction between the alcohol and the solvent that also influences molecular structures. For increased molar concentration the free volume increases as the internal pressure decreases, suggesting the association by bonding hydrogen. This indicates that the interaction of NSB drug with alcohol is increasing. . Relaxation time is decreasing with rising concentration.

CONCLUSION

The ultrasonic study of the liquid mixtures detects a molecular connection arising from the hydrogen bond between the NSB and alcohol molecules.The non-linear change in concentration of thermal acoustic parameters shows the dynamic structure between the component molecules. Ultrasound speed(U), density(Ś) and viscosity (μ) are present in this paper, and acoustic Adiabatic compressibility, frequency, relaxing time, acoustic impendence, attenuation, Rao constant, molar volume, cohesive strength, Wada constant at different concentrations were determined. parameters viz. The parameters shows that, as drug solution concentrations increase and interaction decreases as temperature rises, there is close molecular interactions between different molecules.

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