



**ACOUSTICAL PARAMETERS OF BENZOTHAZOLYL
SUBSTITUTED DERIVATIVES IN BINARY SOLVENT MIXTURES**

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ABSTRACT

Acoustic parameters study of newly synthesised substituted derivatives of benzothiazole were carried out in the present work. Parameter like Density and ultrasonic velocities of different concentrations from 0.01M to 0.000625 M of benzothiazolyl substituted derivatives with of 75%binary solvent mixture i.e. dioxane-water, acetone-water and DMSO-water mixtures were measured at 303.15 K (30oC) by using multifrequency ultrasonic interferometer at frequency 1 MHz and 3 MHz. The density, Concentration and ultrasonic velocity (U) were used to calculate adiabatic compressibility (β_s), intermolecular free length (Lf), relative association (RA) and specific acoustic impedance (Z). The results have been interpreted in terms of solvent-solvent and solute-solvent interactions.

Keywords: Relative association, ultrasonic velocity, Density, molecular interaction

INTRODUCTION

Due to their significant biological and pharmacological properties, heterocyclic compounds analogues and derivatives have attracted a lot of attention in recent years. A heterocyclic compound or ring structure is a cyclic compound that has atoms of minimum two different elements as members of its

ring. Heterocycles play an vital role in biochemical processes because the core groups of the most typical nucleic acids, majority of drugs, essential constituents of the living cells, most biomass and many synthetic and natural dyes are based on heterocycles. For the development of novel

drugs, the benzothiazole moiety has unique and multifunctional properties. Benzothiazole derivatives are found in medicinal and bioorganic chemistry with applications in drug discovery and development for treatment of autoimmune and inflammatory diseases in the prevention epilepsy¹, solid organ transplant rejection, antitumor²⁻⁵, antiviral⁶, anticorrosive⁷, neuroprotective⁸ and immunosuppressive properties.

In recent years the ultrasonic velocity measurement are widely used to understand the nature of molecular interactions existing between liquid mixtures⁹. From the solute-solvent interaction, structure making and breaking properties of liquids have been measured¹⁰⁻¹². Ultrasonic velocity has been suitably employed in understanding the nature of molecular interaction in pure^{13,14}, binary^{15,16} and tertiary mixtures¹⁷. The ultrasonic technology is employed in a wide range of applications in biology, industry, medicine, material science, oceanography, agriculture, sonochemistry etc. because of its non-destructive character.

In the field of agriculture it is utilized widely in chemical additives for getting better the production yield of food. Ultrasonic waves have been useful in the preparation of protein micropheres, biomaterials, in the modification of

polymers and polymer surfaces etc¹⁸⁻¹⁹. A literature review show that scanty of work has been done on benzothiazolyl substituted derivatives in binary liquid mixture with different frequency range. The synthesis of benzothiazolyl substituted derivatives was carried out by microwave technique which was then used for ultrasonic study²⁰⁻²² to determine intermolecular free length L_f , adiabatic compressibility (β_s), specific acoustic impedance (Z), relative association R_A of mixture at different concentration.

EXPERIMENTAL

MATERIALS AND METHOD

In the present study solvent Acetone, dioxan and DMSO of AR grade were used. Substituted benzothiazolyl derivatives (1-Benzothiazol-2-yl-[1,2]diazetidine-3-ylidene)-4(phenyl-thiazole-2-yl)-amine (1c) and (1-Benzothiazol-2-yl-[1,2]diazetidine-3-ylidene)-phenyl-amine (1d) were synthesized by using microwave technique. These derivatives were recrystallised and they were used for the ultrasonic study. All weighing were made by Wensar electronic balance (± 0.001 g). The accuracy measurement was within $\pm 1\%$ Kgm^{-3} . Multi-frequency Ultrasonic interferometer from Mittal enterprises, Model M-83 with accuracy of $\pm 0.03\%$ and frequency 1 MHz and 3 MHz was used for the measurement of ultrasonic velocities of different solutions.

In the present work different thermodynamics parameters such as adiabatic compressibility (β_s), intermolecular free length (L_f), relative association (R_A) and specific acoustic impedance (Z) have been calculated with the help of following equations-

$$u = \lambda x f$$

$$L_f = K \sqrt{\beta}$$

$$\beta = \frac{1}{v} \left[\frac{\partial v}{\partial p} \right]$$

$$\beta = \frac{1}{\rho u^2}$$

$$R_A = \left(\frac{\rho}{\rho_0} \right) \left(\frac{u_0}{u} \right)^{1/3}$$

$$Z = \rho x u$$

RESULTS AND DISCUSSION

Table 1: Acoustic Parameters in 75 % Acetone-Water mixture (Temperature: 30°C; Ultrasonic frequency- 1 MHz and 3 MHz)

Conc. (M)	U/m.s ⁻¹	$\beta/x10^{-10} \cdot m^2 \cdot N^{-1}$	$L_f/x10^{-11} \cdot m$	Z/Kg.m ² s ⁻¹	$R_A/m^3 \cdot mol^{-1}$
Frequency- 1 MHz					
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-4(phenyl-thiazole-2-yl)-amine					
0.01	1381	5.3965	4.7645	1264790	0.985
0.005	1370	5.4636	4.8299	1271681	0.983
0.0025	1363	5.5306	4.8953	1272572	0.982
0.00125	1349	5.6377	4.9408	1273462	0.977
0.000625	1342	5.6747	5.0062	1292353	0.974
1-Benzothiazol-2-l-[1,2]diazetidene-3-ylidene)-phenyl-amine					
0.01	1391	5.5933	4.8106	1211108	0.960
0.005	1388	5.6449	4.9138	1219920	0.957
0.0025	1386	5.7445	4.9266	113733	0.957
0.00125	1382	5.7605	4.9332	114546	0.955
0.000625	1381	5.7997	4.9398	1246358	0.954
Frequency- 3 MHz					
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-4(phenyl-thiazole-2-yl)-amine					
0.01	1400	4.4291	4.3168	1262921	0.995
0.005	1395	4.7947	4.4913	1291042	0.993
0.0025	1388	4.8305	4.508	1336677	0.992
0.00125	1381	5.1445	4.6522	1340481	0.987
0.000625	1380	5.3609	4.7491	1393127	0.984
1-Benzothiazol-2-l-[1,2]diazetidene-3-ylidene)-phenyl-amine					
0.01	1413	4.6281	4.4651	1189180	0.983
0.005	1413	5.7467	4.9756	1199753	0.980
0.0025	1393	6.0522	5.1061	1203133	0.980
0.00125	1388	6.0692	5.1133	1231219	0.978
0.000625	1380	6.1530	5.1484	1373335	0.977

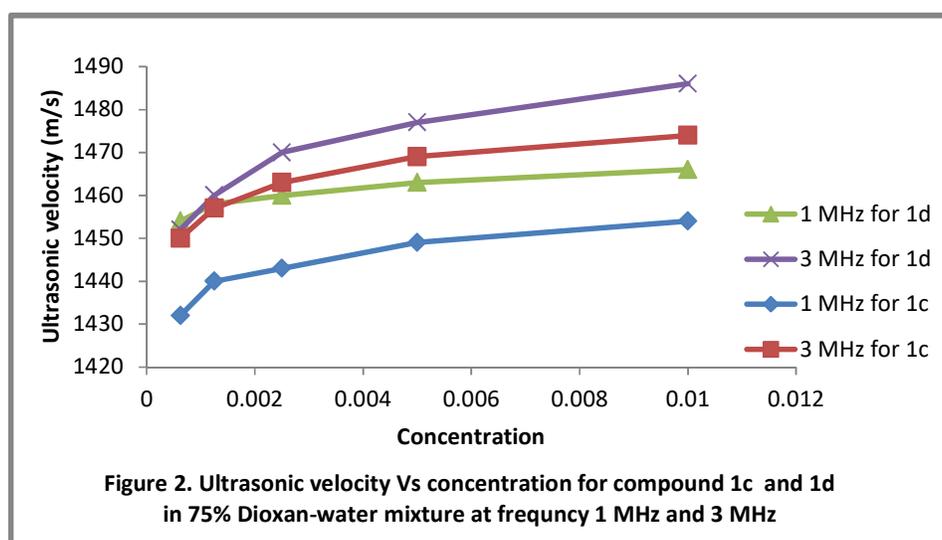
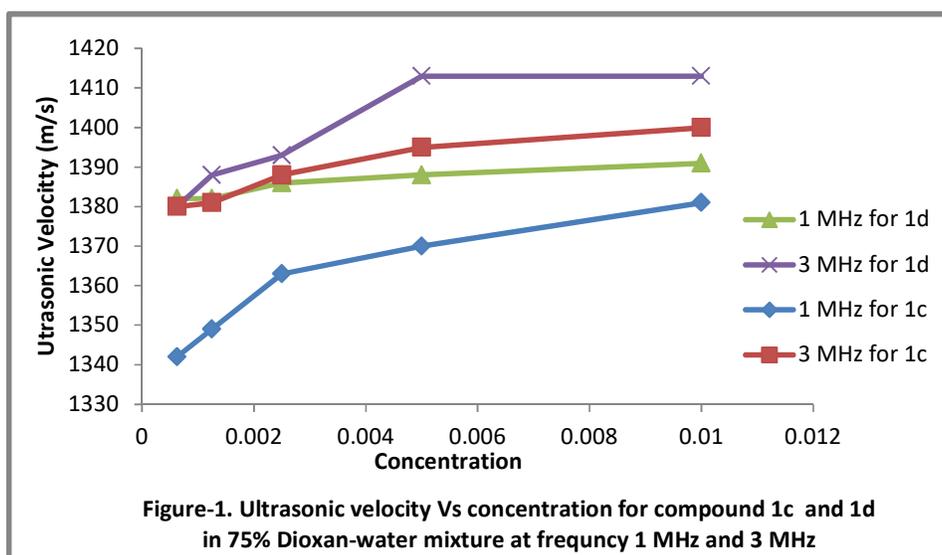
Table 2: Acoustic Parameters in 75 % Dioxane-Water mixture (Temperature: 30°C; Ultrasonic frequency- 1 MHz and 3 MHz)

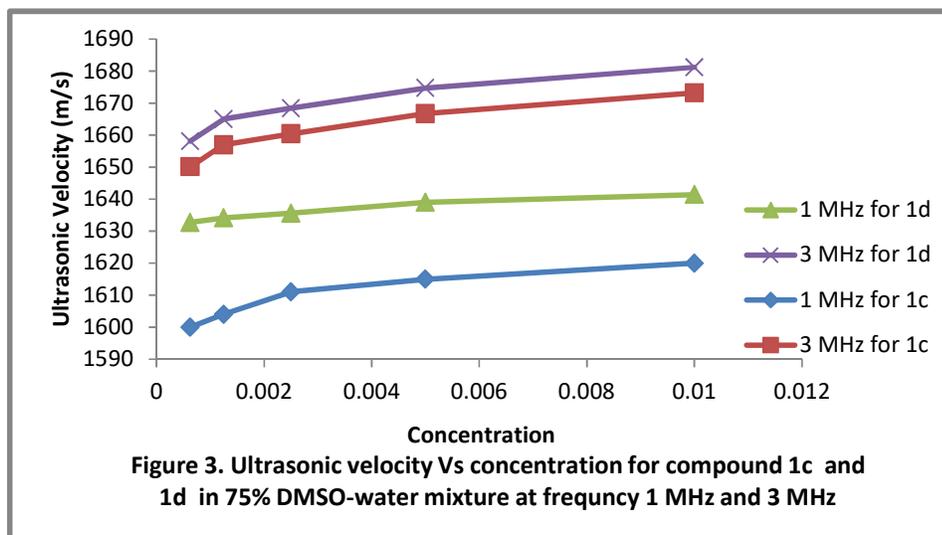
Conc. (M)	U/m.s ⁻¹	$\beta/x10^{-10} \cdot m^2 \cdot N^{-1}$	Lf/x10 ⁻¹¹ .m	Z/Kg.m ² s ⁻¹	R _A /m ³ .mol ⁻¹
Frequency- 1 MHz					
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-4(phenyl-thiazole-2-yl)-amine					
0.01	1454	4.1782	4.1931	1490728.5	0.979
0.005	1449	4.2201	4.214	1499561.7	0.975
0.0025	1443	4.2953	4.2512	1514432.8	0.974
0.00125	1440	4.382	4.2939	1526050.4	0.970
0.000625	1432	4.4262	4.3154	1532206.9	0.967
1-Benzothiazol-2-l-[1,2]diazetidene-3-ylidene)-phenyl-amine					
0.01	1466	4.2264	4.2171	1507712.5	0.986
0.005	1463	4.2658	4.2367	1508066.1	0.984
0.0025	1460	4.3123	4.2596	1511501.2	0.983
0.00125	1458	4.3223	4.2646	1518784.5	0.982
0.000625	1454	4.3319	4.2693	1529717.9	0.981
Frequency - 3 MHz					
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-4(phenyl-thiazole-2-yl)-amine					
0.01	1474	3.9297	4.0668	1435818.9	1.013
0.005	1469	4.0757	4.1414	1490940.7	1.003
0.0025	1463	4.2116	4.2097	1529090.8	0.997
0.00125	1457	4.4256	4.3151	1552161.8	0.989
0.000625	1450	4.7705	4.4799	1581635.0	0.986
1-Benzothiazol-2-l-[1,2]diazetidene-3-ylidene)-phenyl-amine					
0.01	1486	3.9835	4.0945	1510642.4	1.008
0.005	1477	4.0242	4.1153	1546680.4	1.001
0.0025	1470	4.0964	4.1519	1553270.0	1.000
0.00125	1460	4.1142	4.1609	1562715.1	0.997
0.000625	1452	4.3148	4.2609	1569490.8	0.993

Table 3: Acoustic Parameters in 75 % DMSO-Water mixture (Temperature: 30°C; Ultrasonic frequency- 1 MHz and 3 MHz)

Conc. (M)	U/m.s ⁻¹	$\beta/x10^{-10} \cdot m^2 \cdot N^{-1}$	Lf/x10 ⁻¹¹ .m	Z/Kg.m ² s ⁻¹	R _A /m ³ .mol ⁻¹
Frequency- 1 MHz					
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-4(phenyl-thiazole-2-yl)-amine					
0.01	1620.00	2.8360	3.4953	1574636	1.020
0.005	1615.00	3.6267	3.9526	1585748	1.019
0.0025	1611.00	4.1919	4.2495	1614280	1.016
0.00125	1604.00	4.2802	4.2940	1737822	1.002
0.000625	1600.00	4.3432	4.3255	1966254	1.001
1-Benzothiazol-2-l-[1,2]diazetidene-3-ylidene)-phenyl-amine					
0.01	1641.43	2.5723	3.3288	1715929	1.044
0.005	1639.00	2.6391	3.3718	1769639	1.032
0.0025	1635.57	3.2647	3.7502	1832594	1.022
0.00125	1634.14	3.4882	3.8764	2037194	0.989
0.000625	1632.71	3.6554	3.9682	2046069	0.965
Frequency = 3 MHz					
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-4(phenyl-thiazole-2-yl)-amine					
0.01	1673.20	3.3098	2.9490	1787618	1.021
0.005	1666.70	3.0705	3.5810	1820064	1.017
0.0025	1660.40	2.0187	3.6370	1886159	1.016
0.00125	1657.00	2.9769	3.7760	1901462	1.011

0.000625	1650.10	3.3699	3.8101	2329265	1.002
1-Benzothiazol-2-yl-[1,2]diazetidene-3-ylidene)-phenyl-amine					
0.01	1681.20	3.0125	3.2958	1689161	1.031
0.005	1674.70	3.5254	3.6024	1752830	1.028
0.0025	1668.40	2.5216	3.8847	1760276	1.015
0.00125	1665.00	3.5031	3.8970	1907778	1.011
0.000625	1658.10	3.7742	4.0322	2084134	1.000





The calculated values of all parameters are listed in Table 1, 2 and 3. Figure 1, 2 and 3 shows that velocity of the solution increases as concentration increases. The increase in velocity is directly proportional to the molecular weight of the solute. Hence lead to solute-solvent interaction. While increase in frequency 1 MHz to 3 MHz ultrasonic velocity also increases due to molecular interaction in binary liquid mixture.

The ultrasonic velocity (U) for both of the compounds is found to be the lowest at low concentration and the increase in ultrasonic velocity with increase in concentration. This linear increase suggests that there are maximum association among the molecules of mixture and strong solute-solvents interactions in the solution mixture. from the observation table it is reveals that the velocity values are higher in 75% DMSO-water mixture than that of

the 75% Acetone-water and Dioxane-water mixture which may be due to the greater solute-solvent interaction found in 75% DMSO-water system. This is due to the structural differences in 75% DMSO-water, Dioxane-water and Acetone-water.

Adiabatic compressibility (β) values increase with decrease in concentration which may be due to aggregation of solvent molecules around the solute increase in solute-solvent interactions. The increase in intermolecular free length with decrease in concentration is a normal trend. The decrease in compressibility brings the molecules to a closer packing resulting into a decrease of intermolecular free length. As the ultrasonic velocity increase, intermolecular free length decrease and vice-versa. The values of acoustic impedance (Z) in DMSO-water > Dioxane-water > acetone-water system supporting the findings that solute-solvent interactions is

stronger in DMSO-water system. Relative association is the measure of extent of association of component in the medium¹⁵. The relative association value is depends on either the salvation of present ions or breaking up of the solvent molecules on addition of solute to it. Relative association R_A decreases linearly with decrease in concentration. It is influenced by breaking of ions. The values R_A are found to be lower in acetone-water system as compared to dioxane-water and DMSO-water system.

With decrease in concentration the ultrasonic velocity for all the three frequencies (1MHz, and 3 MHz) were decreases. The ultrasonic velocity at different frequency range shows following trend $3\text{MHz} > 1\text{MHz}$

CONCLUSION:

In the present study from the experimental data, It is conclude that in the mixture of studied both of the compounds 1-Benzothiazol-2-yl-[1,2]diazetidine-3-ylidene)-4(phenyl-thiazole-2-yl)-amine (1c) and (1-Benzothiazol-2-yl-[1,2]diazetidine-3-ylidene)-phenyl-amine (1d) solute-solute and solute-solvent interaction is existing. It is observed that the compound (1-Benzothiazol-2-yl-[1,2]diazetidine-3-ylidene)-phenyl-amine (1d) shows strong solute-solvent interaction with binary mixture solvent Acetone-water, Dioxane-water as well as DMSO-Water in two different frequencies at 30°C.

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