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Research Article

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Ultrasonic studies on molecular interaction of substituted thiazolidines in acetone using pulse-echo technique

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ABSTRACT

Velocities of longitudinal ultrasonic waves have been measured at room temperature for substituted thiazolidines in acetone (w:v %) using pulse-echo technique. Data of the measured ultrasonic velocity and density were used to evaluate many acoustical and volumetric parameters, such as specific acoustic impedance, adiabatic compressibility, partial molal volume, intermolecular free length, apparent molal compressibility, relative association and salvation number. The changes in these parameters have been interpreted in terms of acetone concentration. Results showed that, the acoustical and volumetric parameters yielded valuable information about the behavior of acetone in the investigated solutions of thiazolidines.

Key words: Thiazolidines, ultrasonic velocity, adiabatic compressibility.

INTRODUCTION

It has been noticed over the years that interesting biological activities were associated with thiazolidines. Recently applications of thiazolidines were found in drug development for the treatment of allergies, [1] HIV infections, [2] tumor, [3] bacterial and inflammation. [3,4] Aly *et al* have recently reported on the synthesis of various selected thiazolidines of antibacterial and antioxidant activities. [5,6] In the recent years, the ultrasonic non-destructive pulse-echo technique has been found to be one of the best techniques to characterize the acoustical properties of materials. The measurements of the ultrasonic velocity are helpful to interpreted solute-solvent, ionsolvent interaction in aqueous and non aqueous medium. [7-9] Fumio *et al* [10] studied the acoustical properties of complex in water. It was investigated the acoustical properties of four different drugs in methanol and/or water and it was drawn conclusion from adiabatic compressibility. [11,12] Meshram *et al* also studied the different acoustical properties of some substituted pyrazolines in binary mixture acetone-water and observed variation of ultrasonic velocity with concentration. [13] In other site, Palani measured both ultrasonic velocity and density of amino acid in aqueous magnesium acetate at constant temperature. [14] It was found that the ion-dipole interaction mainly depends on ion size and polarity of solvent. The strength of ion-dipole attraction is directly proportional to the size of the ions, magnitude of dipole. However that inversely proportional to the distance between ion and molecules. [15] The acoustical and thermodynamic properties of citric acid in water at different temperature. [16] Mishra *et al* have investigated ultrasonic velocity and density in non aqueous solution of metal complex and evaluate acoustic properties of metal complex. [17] Arvinthraj *et al* have determined the acoustic properties for the mixture of amines with amide in benzene at 303K-313K. They also determined thermodynamic parameters 13.S.K. [18] Thakur *et al* have studied the different acoustical parameters of binary mixture of 1-propanol and water. [19] After review of literature survey the detail study of substituted heterocyclic drugs under identical set of experimental condition is still lacking. It was thought of interest to study the acoustical properties of prospective thiazolidines drugs under

suitable condition. Therefore, the goal of the present work is to measure the room temperature ultrasonic velocity for substituted thiazolidines, prepared as reported in literature, [5,6] in acetone (w/v)% as a solvent using pulse-echo technique. The data of measured velocity and density will be used to evaluate many acoustical and volumetric parameters, such as the specific acoustic impedance, adiabatic compressibility, intermolecular free length, apparent molal compressibility, relative association and salvation number.

EXPERIMENTAL SECTION

The substituted thiazolidines, [5,6] are used in the present study. Acetone is used for solution preparation of different drugs. The densities (d_s) of the investigated solutions were determined by using specific gravity bottle. The relative error in these measurements was about ± 1x10^{-4} g/cm^3.

The measurement of ultrasonic velocity (U_s) in each investigated liquid sample was carried out at room temperature and at 2 MHz frequency by using pulse- echo technique (GE model: USN60). The elapsed time between the initiation and the receipt of the pulse was determined. The velocity was therefore obtained by dividing the round trip distance by the elapsed time. The temperature of the solution was mentioned constant by circulating water through the double wall measuring cell made up of glass. Simple combinations of the measured ultrasonic velocity and density allows the determination of the various acoustic and volumetric properties according to the following standard relations:

Specific acoustic impedance $Z = d_s U_s$ (1)

Adiabatic compressibility $\beta_s = \left(\frac{1}{d_s U_s} \right)$ (2)

Intermolecular free length $L_f = K\beta_s^{1/2}$ (3)

where K is Jacobson constant,[7-9] which is given at temperature T by the relation $K = (91.368 + 0.3565T)10^{-8}$. Acetone conc.(%) are expressed by mL: mg (acetone: mg) to give total of one hundred. Accordingly, high concentration of the compound is found, at 55% of it (45 mL of acetone).

RESULTS AND DISCUSSION

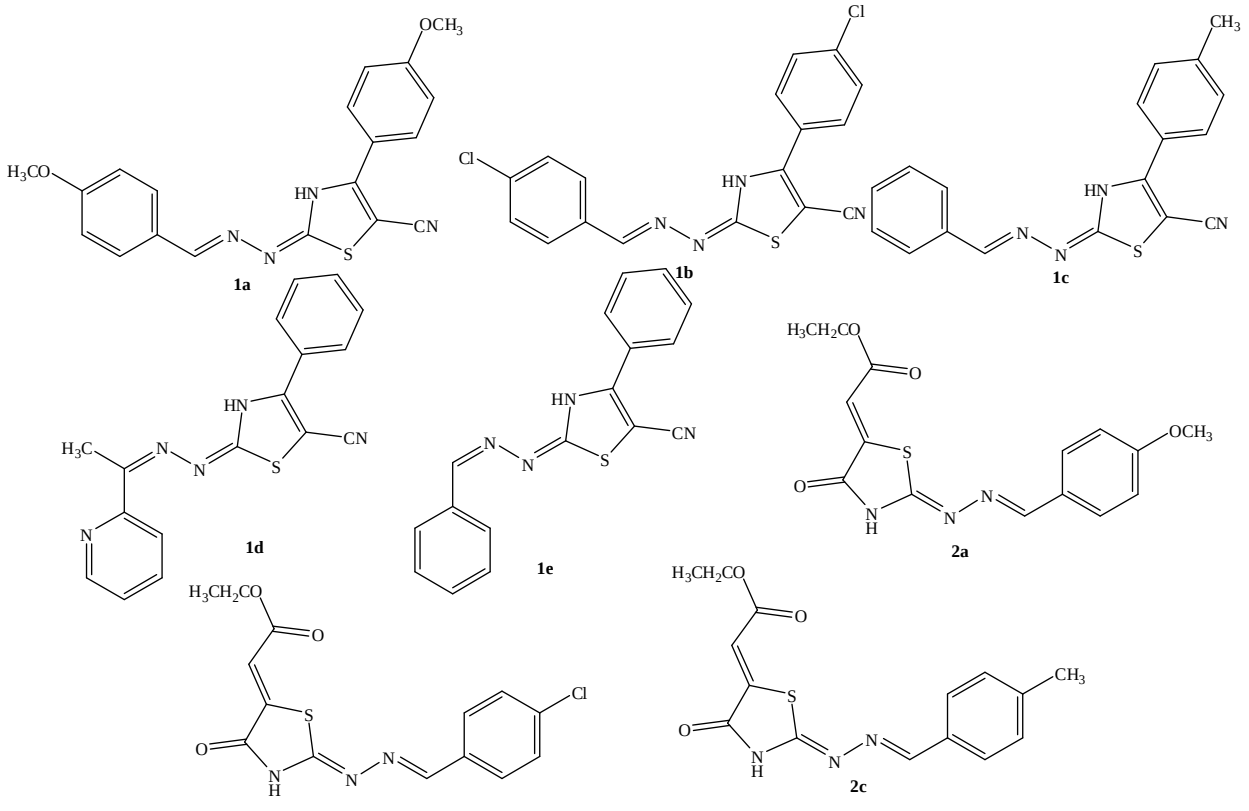


Figure 1. Structures of selected thiazolidines 1a-e and 1a-c

Ultrasonic parameters of selected thiazolidines **1a-e** and **2a-c** (Figure 1) were measured e.g. density (d) and ultrasonic velocity (U_s), are listed in Table 1 for all solutions under investigation, beside the calculated values of adiabatic compressibility (β_s), partial molal volume (f_v), intermolecular free length (L_f), apparent molal compressibility (f_k), specific acoustic impedance (Z), relative association (R_A), solvation number (S_n). It is seen from the table that all the parameters are strongly dependent upon the concentration of acetone in the solution.

It is well known that, the ultrasonic waves travel more faster in a more dense materials. This is true in case of the investigated solutions as shown in Table 1. Figure 2 illustrates how the ultrasonic velocity varies with the concentration of acetone in all solutions under investigation. The figure shows clearly that, the ultrasonic velocity decreases linearly with increasing concentration of acetone in the solution. The changes in the ultrasonic velocity can be explained on the basis of a model presented by Eyring and Kincaid [20] for sound propagation as follows. According to this model, variation of ultrasonic velocity in solution depends upon the increase or decrease of intermolecular free length after mixing the components. Generally, it is expected that the intermolecular free length and ultrasonic velocity should show a inverse relation with each other. It has been found that, increasing the concentration of the substituted heterocyclic compounds in dioxane leads to an increase in the intermolecular free length and decrease in the measured ultrasonic velocity. The increase in the intermolecular free length to the greater force of interaction between solute and solvent by forming hydrogen bonding. [20] This is due to the significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the added electrolyte. This may also indicates that decrease in number of free ions showing the occurrence of ionic association due to weak ion-ion interaction. In case of the investigated solutions, the behavior of the intermolecular free length with the percentage of acetone is completely opposite to that of the measured ultrasonic velocity. These results prove that Eyring and Kincaid model [20] is valid for the investigated solutions. Equation (1) suggests that the acoustic impedance of materials depend on two major parameters, which are the density and ultrasonic velocity.

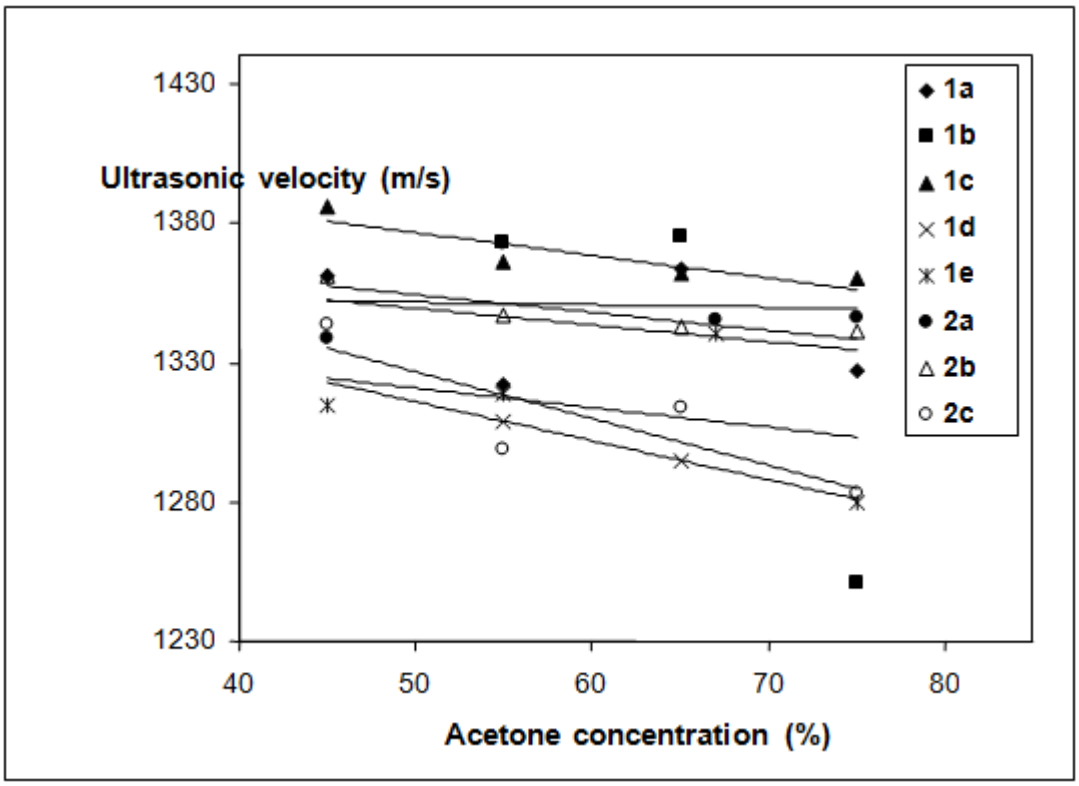


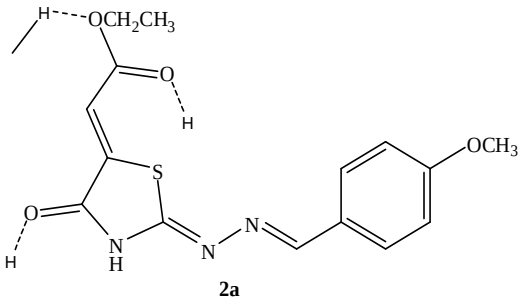
Figure. 2: Variation of ultrasonic velocity with acetone concentration for the substituted thiazolidines 1a-e and 2a-c in acetone-water mixture. The solid lines are drawn as a guide to the eye.

One interesting observation in Table 1 is that, the measured density values changes slightly with increasing the acetone concentration in all studied solutions. This suggests that ultrasonic velocity is the controlled factor for estimating the acoustic impedance of these solutions. This suggests that ultrasonic velocity is the controlled factor for estimating the acoustic impedance of these solutions. This explains why the acoustic impedance behave the same trend as that of ultrasonic velocity with acetone concentration. Generally, it is expected that the acoustic impedance

and adiabatic compressibility should show opposite behavior to each other. This is also true in case of the investigated systems as shown in Table 1. The decrease in the specific acoustic impedance and an increase of adiabatic compressibility with the increase of percentage of acetone in the solution may be due to collection of solvent molecule around ions. This behavior indicates the existence of weak ion-solvent interaction [21] and indicates that there is significant solute-solvent interaction.

Table 1. Ultrasonic velocity, density, adiabatic compressibility and specific acoustic impedance Intermolecular free length of solutions with different percentage of acetone-water mixture.

Acetone conc.(%)	Ultrasonic velocity(m/s)	Density (Kg/m^3)	Adiabatic compressibility ($x10^{-10}Kg/ms^2$)	Intermolecular free length ($x10^{-11}m$)	Acoustic impedance ($x10^6Kg/m^2s$)
1a					
45	1361.23606	813.92	6.64	5.09	1.1071
55	1322.06287	813.76	7.03	5.03	1.0758
65	1363.63636	813.65	6.60	5.08	1.1095
75	1326.97807	813.7	6.98	5.24	1.0798
1b					
55	1373.32281	814.1	6.51	5.04	1.1180
65	1375.49407	814.46	6.49	5.03	1.1203
75	1251.12	816.52	6.82	5.53	1.0216
1c					
45	1386.454	814.12	6.39	5.00	1.1287
55	1366.045	809.53	6.62	5.08	1.1059
65	1362.835	811.52	6.63	5.09	1.1060
75	1359.906	813.79	6.64	5.09	1.1067
1d					
55	1308.763	815.42	7.16	5.29	1.0672
65	1295.004	811.1	7.20	5.26	1.0504
75	1325.462	810.29	7.35	5.36	1.074
1e					
45	1315.441	817.43	7.07	5.25	1.0753
55	1319.181	817.35	7.03	5.24	1.0782
65	1340.008	815.35	6.83	5.16	1.0926
75	1280.471	816.61	6.47	5.40	1.0456
2a					
55	1373.323	808	6.56	5.06	1.1096
65	1344.928	812	6.81	5.16	1.0920
75	1346.489	813	6.78	5.15	1.0947
2b					
55	1346.749	813	6.78	5.15	1.0949
65	1342.852	810	6.85	5.17	1.0877
75	1340.524	810	6.87	5.18	1.0858
2c					
55	1299.235	809	7.32	5.35	1.0511
65	1314.199	807	7.17	5.29	1.0606
75	1283.422	806	7.53	5.42	1.0344



2a

Figure 3. Suggested hydrogen bond formation in compound 2a

In Table 1, it is also cleared that high intermolecular length was appeared in **1d** compared with other substituents, suggested that increasing its hydrogen bond interaction in solution. It is well-known that biological activity of chemical compounds depend on the presence of intermolecular hydrogen bond (IHB). [22] Thus, it can be noted that compound **1d** would show potentially high biological activity as compared with the other substituents due to the basicity pyridine moiety. [5] From Besides, it can be also concluded that high dilution of the organic moiety (75%

acetone) increases with the intermolecular free length, so that more increasing of the hydrogen bond formation. Thus, it can be noted that compound **1d** would show potentially high biological activity as compared with the other substitutents due to the basicity pyridine moiety. [5] Besides, it can be also concluded that high dilution of the organic moiety (75% acetone) increases with the intramolecular free length, so that more increasing of the hydrogen bond formation. It is obviously noted that compounds **2a-c** contain three oxygen atoms as electronegative elements that enable to hydrogen bond formation (e.g. compound **2a**, Figure 3) with the solvent and consequently indicate high interamolecular lengths compared with those in **1a-e** at more dilutions. It is known that the ultrasonic sound wave causes oscillations in pressure but the oscillations are fast enough that heat can't move from compressed regions to rarified regions in order to keep the temperature constant. Before the heat can be conducted away from the compressed regions the compression has moved on so that sound propagation is adiabatic.

Although static measurements have been used for this purpose, the observations indicated that measurements of protein dynamics are effectively a more "sensitive" method of determining the conditions under which proteins are most stable. [23] Accordingly, measurement of adiabatic compressibility, herein, would give information about the stability of thiazole moiety as a prospective drug against degradation. Moreover, and from Table-1 it is noted that generally, density and ultrasonic velocity increases with increase in molar solution. The increase in velocity is due to the decrease in adiabatic compressibility of the liquid solution. The adiabatic compressibility are the deciding factors of the ultrasonic velocity in the liquid solution which directly relates with the anti-bacterial activity of that compound. More solution concentration of solution more active is the compound towards bacteria hence as the concentration increases activity increases which relates with the effect of adiabatic compressibility of the compound. Hence adiabatic compressibility values is inversely proportional to the molar solution concentration.

CONCLUSION

In conclusion, acoustical and volumetric parameters using ultrasonic echo technique can give us valuable information about the behavior of thiazolidines in solutions of the solute-solvent interaction. Therefore much more studies are required to apply the aforesaid study to various heterocycles in order to study their stability in solutions and to introduce information about their stabilities in solutions to be used as potentially biological active compounds.

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REFERENCES

[1] L. Racane, V. Tralic-Kulenovic, L.F. Jakic, D. W. Boykin, G. Karminski-Zamola, *Heterocycles*, **2001**, *55*, 2085-2098
[2] A. A. Aly, A. B. Brown, M. Abdel-Aziz, G. El-Din A. A. Abuo-Rahma, M. F. Radwan, M. Ramadan, A. M. Gamal-Eldeen *J. Heterocycl. Chem*. **2012**, *49*, 726–731.
[3] B. S. Holla, K. V. Malini, B. S. Rao, B. K. Sarojini, N. S. Kumari *Eur. J. Med. Chem.*, **2003**, *38*, 313–318
[4] N. C. Desai, V. V. Joshi, K. M. Rajpara, H. V. Vaghani, H. M. Satodiya *J. Fluorine Chem.*, **2012**, *142*, 67–78
[5] A. A Aly, E. A. Ishak, T. El Malah, A. B. Brown, W. M. Elayat, *J. Heterocycl. Chem.*, **2013** (submitted).
[6] A. A Aly, E. A. Ishak, A. B. Brown, W. M. Elayat, *J. Sulf. Chem.* **2013** (submitted)
[7] S. Baluja, S. Oza, *Fluid phase equlibria*, **2005**, *200*, 49-54.
[8] M. K. Rawat, Sangeeta, *Ind. J. pure Appl. Phy*. **2008**, *46*, 187-192.
[9] A. Ali, A. K. Nain, *Acoustics Lett*. **1996**, *19*, 53-57.
[10] H. Ogawa, S. J. Murakami *J. Solution. Chem*. **1987**, *16*, 315-318.
[11] F. Kawaizumi, K. Matsumoto, H. Nomura *J. Phys. Chem.* **1983**, *87*, 3161-3166.
[12] D. V. Jahagirdar , B. R. Arbad , S. R. Mirgane, M. K. Lande, A. G. Shankarvar *J.Molecular Liq.* **1998**, *75*, 33-43.
[13] Y. K. Meshram, M. L. Narwade *Acta Ciencia Indica* **2001**, *XXVII.C*, 67-70.
[14] R. Palani, S. Saravanan *Research J. Phy*. **2008**, *2*, 13-21.
[15] V. K. Syal, A. Chauhan, S. Chauhan *J. Pure Ultrasound*. **2005**, *27*, 61-69.
[16] A. Tadkalkar, P. Pawar, G. K. Bichile *J. Chem. Pharm. Res*. **2011**, *3*, 165-168.
[17] A. P. Mishra, D. K. Mishra, *J. Chem. Pharm. Res*. **2011**, *3*, 489-492.
[18] M. Arvinthraj , S. Venktesan, D. Meera, *J. Chem. Pharm. Res*, **2011**, *3*, 623-627.
[19] S. K. Thakur, S.Chauhan, *J. Chem. Pharm. Res*., **2011**, *3*, 657-661.
[20] H. Eyring, J. F. Kincaud, *J. Chem. Phys*, **1938**, *6* ,620-629.
[21] J. D. Pandey, A Shukla , R. D. Rai, K. J. Mishra , *J. Chem. Eng. Data*.,**1989**, *34*, 29-32.
[22] *Intermolecular Interactions: From Diatomics to Biopolymers*, B. Pullman, Ed., New York, 1978

[23] J. D. Ramsey, M. L. Gill, T. J. Kamerzell, E. S. Price, S. B. Joshi,S. M. Bishop, C. N. Oliver, C. R. Middaugh, *J Pharm Sci.* **2009**, *98*, 2432–2447.