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Study of Molecular Interactions in Aqueous 2-Amino-5-Nitrothiazole-$NiCl_2$ Solution at Different Temperatures and Concentrations

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Abstract

Ultrasonic velocity and density of aqueous 2-amino-5-nitrothiazole – $NiCl_2$ solution was guarded at different temperatures (303.15 K, 308.15 K, 313.15 K and 318.15 K) and concentrations, so as to know about the molecular interaction between solute and solvent. In these studies acoustical parameters such as intermolecular free length, isentropic compressibility, specific acoustic impedance, relative association and ultrasonic velocity number were used to interpret types of molecular interactions present in the aqueous 2-amino-5-nitrothiazole -$NiCl_2$ solution of different concentrations at different temperatures. Measured values indicate the presence of effective correlation in the form of solute - solvent interactions and metal-ligand interactions for different concentration and temperature.

***Keywords:** Molecular interactions; 2-amino-5-nitrothiazole; $Nicl_2$; Acoustical parameters*

Introduction

This study is the continuation of our earlier work [1-3] on acoustical study of substituted thiazole in various solvents with varying temperature and concentration. In this study 2-amino-5-nitrothiazole is a Sulfur and Nitrogen containing heterocyclic compound which has vast application in therapeutic chemistry, biological process and industrial process which provide the idea about life process/ mean [4]. Physicochemical properties of the systems can be determined from information of density, ultrasonic velocity and various acoustical parameters. Valuable information like complex formation, molecular association, internal pressure, internal structure etc. can be obtained from the study of molecular interaction. How easily molecules can slide over one another during their flow determines flow rate of liquid and nature of the substance present in the solution.

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Measurement of acoustical study of organic ligand solutions with metal solutions provide excellent information regarding solute- solvent and solute-solute i.e. metal - ligand interaction and structure breaking and making properties of solutes. Acoustical parameters such as ultrasonic velocity, density, relative association, acoustical impedance etc. of 2-amino-5-nitrothiazole-$NiCl_2$ in aqueous solution at different temperature and concentrations measured in this investigation was lacking and therefore present work is undertaken to study acoustical parameters at different temperature and concentration in order to know the effect of temperatures and concentrations on acoustical parameters. The applications of 2-amino-5-nitrothiazole in different areas of science makes our interest in the computation of their acoustical properties so as to know the solute – solvent and solute – solute interaction at different temperature and concentrations.

Materials and Methods

The solvents i.e. water used in this investigation were purified by using $KMnO_4$ and NaOH through double distillation. The ligand 2-amino-5-nitrothiazole (Hi-MEDIA, minimum wt. 97%), used are of synthesis grade. The ligand and metal solutions in water were prepared by dissolving an accurate amount in an aqueous solvent in standard flask with airtight caps and the mass measurement were performed using high precision digital balance (Adair Datta of accuracy ± 0.01 mg). The ultrasonic velocities 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solutions of different concentration were measured by ultrasonic interferometer (Mittal enterprises, model F-81s) at 2 MHz having accuracy ± 1 $m \cdot s^{-1}$ in velocity. It consists of high frequency generator and a measuring cell. The densities of experimental solutions measured by using digital density meter (Anton Paar DMA 35 of accuracy ± 0.001). A thermostatically controlled well-stirred water bath whose temperature was controlled to ± 0.1 K was used for all the measurements.

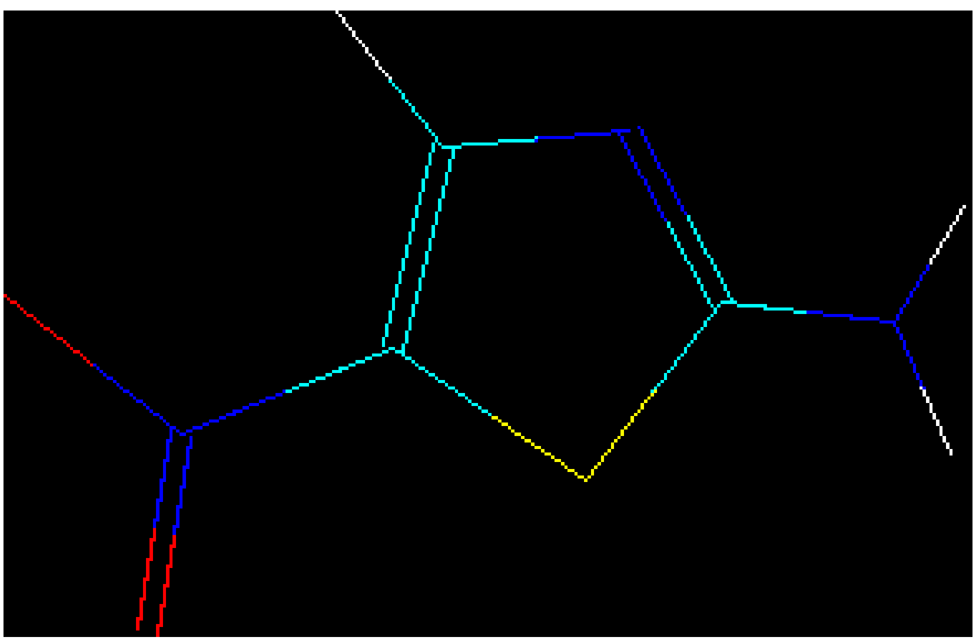

FIG. 1. **Structure of 2-amono-5-nitrothiazole.**

Experimental Theory

Numerous methods are available in the literature for measuring ultrasonic velocity in solid and liquids. The ultrasonic interferometer is considered as more reliable and precise instrument. The expression used to determine ultrasonic velocity using ultrasonic interferometer is:

$$u = v\lambda \qquad (1)$$

Where u is ultrasonic velocity and λ is wavelength.

The isentropic compressibility β_s was calculated from following equation:

$$\beta_s = 1/\rho u^2 \qquad (2)$$

Where ρ is density of solution and *u* is speed of ultrasonic velocity.

The intermolecular free length L_f is calculated by using the standard expression:

$$L_f = K\, \beta_s^{1/2} \qquad (3)$$

Where K is temperature dependent constant known as a Jacobson constant [5].

The acoustic impedance Z is obtained by equation:

$$Z = u\rho \qquad (4)$$

The relative association R_A was calculated by the following equation:

$$R_A = (\rho/\rho_o)\,(u_o/u)^{1/3} \qquad (5)$$

Where ρ_o is density of solvent and u_o is velocity of solvent. Also the sound velocity number is calculated from following equation;

$$[U] = u\text{-}u_o/u_o c \qquad (6)$$

[U] is sound velocity number; c is concentration of the solute.

Results and Discussion

The measured values of ultrasonic velocities and densities for 2-amino-5-nitrothiazole-$NiCl_2$ (FIG. 1) aqueous solution at temperatures (303.15 K, 308.15 K, 313.15 K and 318.15 K) listed in TABLE 1, drawn in FIG. 2 and FIG. 3. From FIG. 2 it is observed that the values of density increased as the concentration of 2-amino-5-nitrothiazole increases & same with temperature. From FIG. 3 it is observed that the values of ultrasonic velocity increases with increase in concentration of 2-amino-5-nitrothiazole, this indicates the association of molecules in the experimental solution [6]. This may be due to dipole-dipole interactions and intermolecular hydrogen bonding between solute and solvent molecules. More number of monomeric water molecules is formed due to breaking down of hydrogen bonding between water molecules with increase in temperature. Monomeric water molecules get trapped in the vacant position present in the cage like structure of water molecules [7]. Due to addition of 2-amino-5-nitrothiazole to the aqueous $NiCl_2$ the interaction between water and $NiCl_2$ decreases as a result lowering of compressibility between molecules in the solutions. This result, polar molecules of 2-amino-5-nitrothiazole forms more compact structure with the water molecule through intermolecular hydrogen bonding [8]. The solution is predominantly composed of water-water interaction which forms the typical three dimensional cage-like structure of water and increase in association observed in the experimental solutions due to water structure enhancement brought by an increase in electrostriction/ means in presence of $NiCl_2$ [7], due to which increase in ultrasonic velocity takes place.

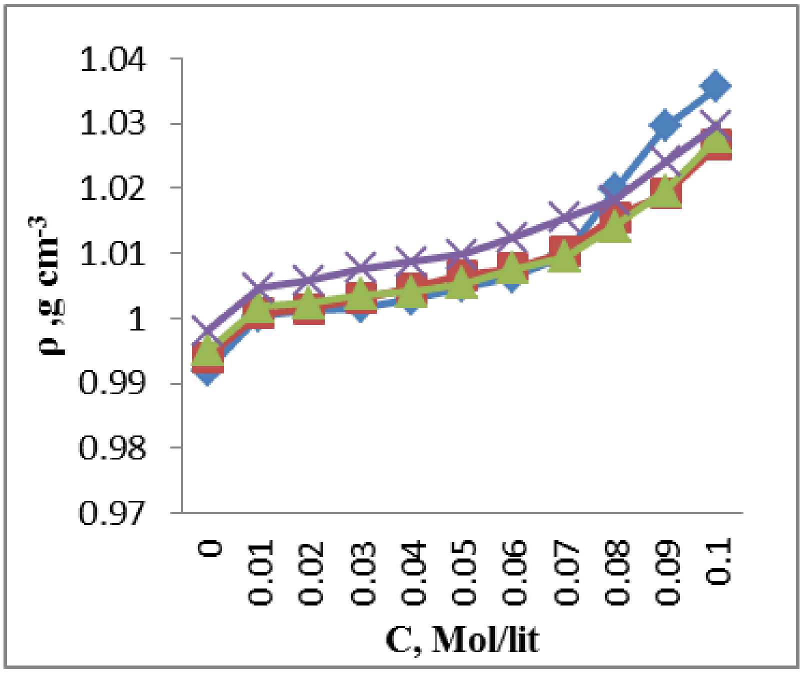

FIG. 1. **Density (ρ) plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (♦), 308.15 K (■), 313.15 K (▲), 318.15 K (×).**

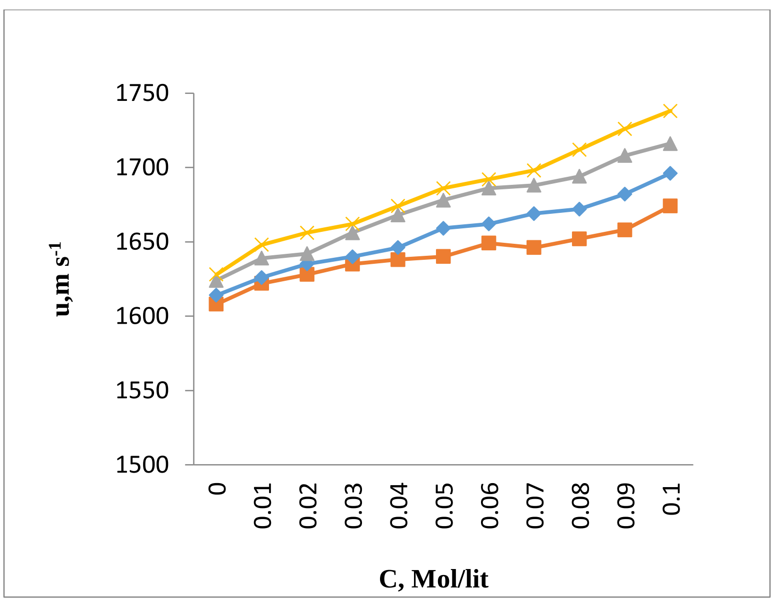

FIG. 2. **Ultrasonic velocity (u) plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (■), 308.15 K (♦), 313.15 K (▲), 318.15 K (×).**

When ultrasonic waves incident on the solution, the molecules get perturbed. The reason is medium has some elasticity and due to this perturbed molecules regain their equilibrium positions [9]. When a solute is added to a solvent, its molecules attract certain solvent molecules toward them; this phenomenon is known as compression. Every solvent has a limit for compression and is known as limiting compressibility. The compressibility of the solution is lowers than that of solvent due to the increase in volumetric concentration of solution with decrease in compressibility of the solution. However the electrostrictive forces cause breakage in the structure of water with increase in solute concentration and compact packing occurs with the water molecules surrounding the solute due to which reducing of compressibility occurs. From FIG. 4 it is observed that the isentropic compressibility for 2-amino-5-nitrothiazole- $NiCl_2$ aqueous solution decreases with increase in the 2-amino-5-nitrothiazole concentration and temperature. This indicate the existence of strong solute- solvent interaction through dipole-dipole and acceptor – donor interactions of the $–NH_2$ group of 2-amino-5-nitrothiazole with surrounding water molecules [9,10].

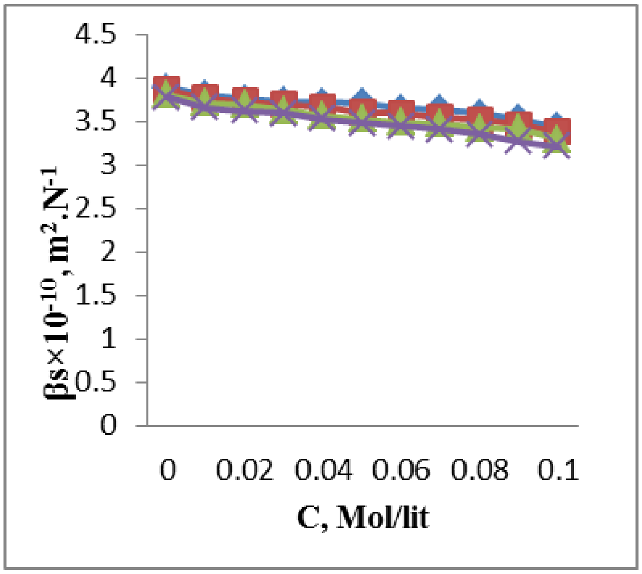

FIG. 4. **Isentropic compressibility (βs) plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (♦), 308.15 K (■), 313.15 K (▲), 318.15 K (×).**

From FIG. 5 it is observed that the intermolecular free length decreases which indicates closer packing [7]. Variation of ultrasonic velocity in a solution depends on the intermolecular free length on mixing. On the basis of a model for sound propagation given by Erying and Kincaid [11], ultrasonic velocity increases with decrease of free length (L_f) and vice versa. Intermolecular free length is a predominant factor for determining the variation of ultrasonic velocity in liquids and their solutions [12]. Intermolecular free length (L_F) is the distance between the surfaces of the neighboring molecules and indicates a significant interaction between solute–solvent as well as metal-ligand [13] suggesting a structure promoting tendency of 2-amino-5-nitrothiazole-$NiCl_2$ in aqueous solution [14]. When the ultrasonic wave travels through a solution, some part of it travels through the medium and remaining part of ultrasonic wave gets reflected by the solute [15] it means solutes restricts free flow of sound wave. The character that decreases this restriction or backward movement of sound waves is known as acoustic impedance (Z). The specific acoustic impedance is dependent on both concentration and temperature of the solution. As the internal pressure and cohesive energy [16] increases with solute concentration, strong intermolecular hydrogen bonding occurs between 2-amino-5-nitrothiazole and water molecule. Hence, an increase in specific acoustic impedance is caused by an increase in instantaneous pressure exert at any molecule (2-amino-5-nitrothiazole - $NiCl_2$ in aqueous solution) with propagation of a sound wave (FIG. 6). It is to be noted that the Ni–2-amino-5-nitrothiazole complex is formed by bonding between Ni (II) and the amino group of 2-amino-5-nitrothiazole [17,18]. FIG. 7 shows that the relative association (R_A) increases with increase in temperature and the increase of concentration of 2-amino-5-nitrothiazole. This is due to the solute-solvent interaction and metal -ligand interactions. It depends on either the breaking up of the solvent molecules on addition of solute molecules in solvent at certain temperature or the solvation of ions that are present [19,20].

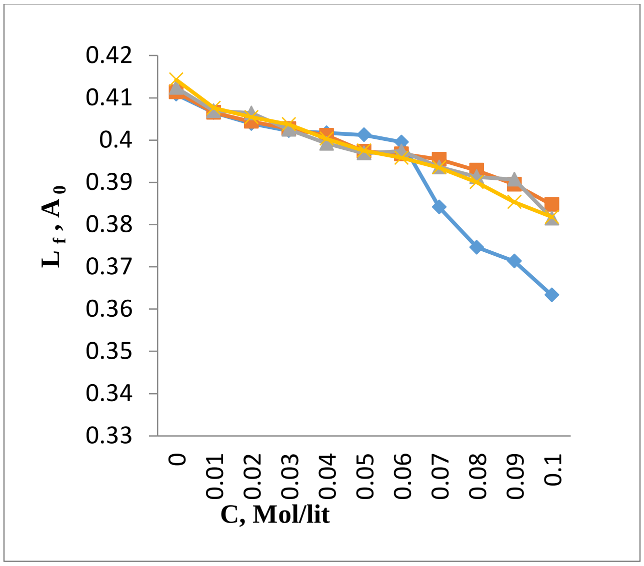

FIG. 3. **Linear free length (L_f) Isentropic compressibility (βs) plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (♦), 308.15 K (■), 313.15 K (▲), 318.15 K (×).**

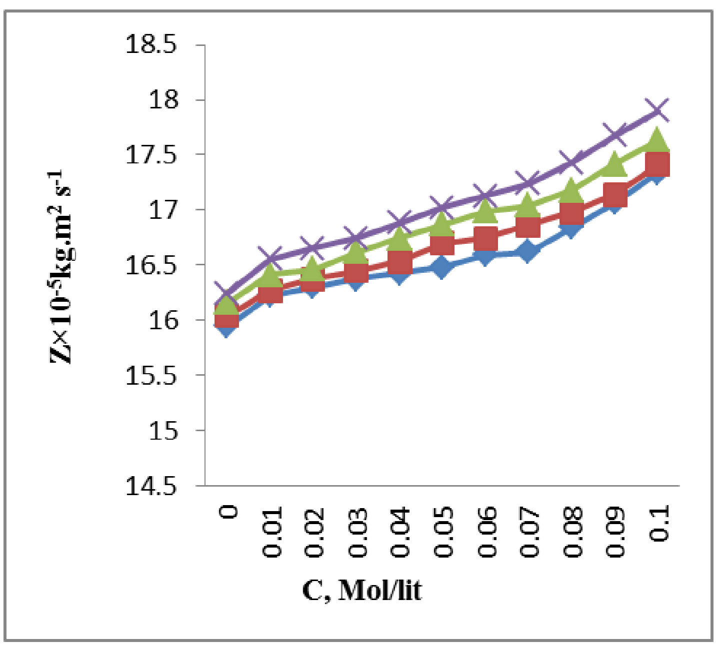

FIG. 6. **Specific acoustic impedance plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (♦), 308.15 K (■), 313.15 K (▲), 318.15 K (×).**

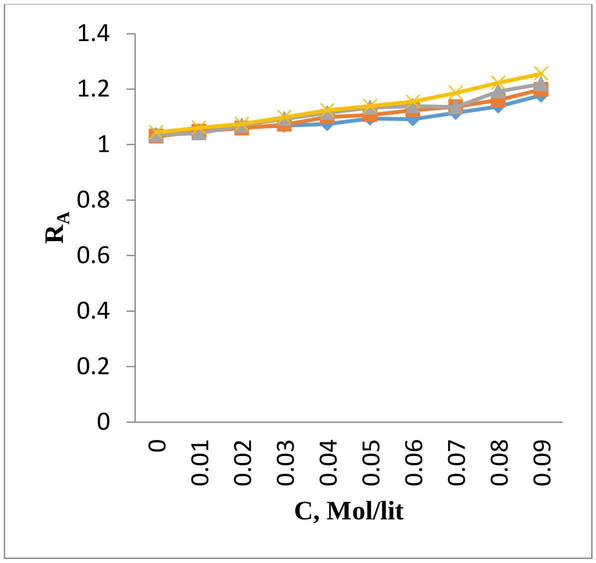

FIG. 4**. Relative association (RA) plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (♦), 308.15 K (■), 313.15 K (▲), 318.15 K (×).**

In general sound velocity number increases with increase in concentration of solute [21] and increase in temperature, however in present investigation there is first decrease in sound velocity number with increase in concentration but after some interval of increase in concentration, U remain constant (FIG 8). Again sound velocity number increase as temperature goes on increases (TABLE 2).

TABLE 1. **Density (ρ) and ultrasonic velocity (u) values for 2-amino-5-nitrothiazole – $NiCl_2$ aqueous solution at different concentrations and temperatures.**

C, m/lit		ρ ,kg m^{-3}				u, m s^{-1}		
	303.15 K	308.15 K	313.15 K	318.15 K	303.15 K	308.15 K	313.15 K	318.15 K
0.00	0.992	0.994	0.995	0.998	1608.01	1614.02	1624.06	1628.01
0.01	1.0003	1.0007	1.0018	1.0046	1622.06	1626.04	1639.02	1648.02
0.02	1.0013	1.0015	1.0024	1.0058	1628.02	1635.08	1642.03	1656.09
0.03	1.0016	1.0031	1.0036	1.0076	1635.03	1640.02	1656.08	1662.01
0.04	1.0029	1.0046	1.0041	1.0086	1638.02	1646.06	1668.02	1674.02
0.05	1.0048	1.0067	1.0053	1.0098	1640.07	1659.06	1678.06	1686.02
0.06	1.0063	1.0076	1.0076	1.0124	1649.06	1662.01	1686.08	1692.03
0.07	1.0097	1.0103	1.0094	1.0154	1646.09	1669.03	1688.04	1698.08
0.08	1.0198	1.0156	1.0142	1.0182	1652.05	1672.04	1694.06	1712.05
0.09	1.0296	1.0192	1.0196	1.0241	1658.06	1682.08	1708.06	1726.02
0.01	1.0356	1.0267	1.0278	1.0297	1674.08	1696.04	1716.08	1738.04
Uncertain ties in temperature, density and velocity are 0.1 K,1 m s^{-1} and 0.0005 k g m^{-3}								

TABLE 2**. Values isentropic compressibility (βs), Relative association, Specific acoustic impedance, linear free length and sound velocity number for 2-amino-5-nitrothiazole – $NiCl_2$ aqueous solution at different temperature and concentrations.**

C, mol/lit	**$\beta s\times10^{-10}$, $m^2.N^{-1}$**	**R_A**	**$Z\times10^{-5}$kg. m^2 s^{-1}**	**L_f , A_0**	**[U], kg mol^{-1}**
At 303.15 K					
0.00	3.89	-	15.951	0.4108	-
0.01	3.81	1.035081	16.225	0.4065	0.8737
0.02	3.76	1.047478	16.301	0.4039	0.6221
0.03	3.73	1.061595	16.376	0.4022	0.5601
0.04	3.72	1.06882	16.427	0.4017	0.4665
0.05	3.71	1.074872	16.479	0.4012	0.3987
0.06	3.65	1.094112	16.594	0.3795	0.4254
0.07	3.64	1.092057	16.621	0.9741	0.3383
0.08	3.59	1.114944	16.847	0.3946	0.3423
0.09	3.53	1.137913	17.071	0.3913	0.3458
0.10	3.44	1.178058	17.336	0.8633	0.4108
At 308.15 K					
0.00	3.86	-	16.043	0.4114	-
0.01	3.77	1.029384	16.271	0.4065	0.7447
0.02	3.73	1.047518	16.375	0.4044	0.6524
0.03	3.70	1.058806	16.451	0.4027	0.5369
0.04	3.67	1.072103	16.536	0.4011	0.4962
0.05	3.60	1.100044	16.701	0.3973	0.5581
0.06	3.59	1.106814	16.746	0.3967	0.4955
0.07	3.55	1.123938	16.862	0.9454	0.4868
0.08	3.52	1.136244	16.981	0.3928	0.4493
0.09	3.46	1.160689	17.143	0.3895	0.4685
0.10	3.38	1.198541	17.413	0.3847	0.5081
At 313.15 K					
0.00	3.81	-	16.159	0.4124	-
0.01	3.71	1.034915	16.419	0.4069	0.9211
0.02	3.70	1.041250	16.459	0.4064	0.5532
0.03	3.63	1.069486	16.620	0.4025	0.6572

0.04	3.57	1.093330	16.748	0.3992	0.6766
0.05	3.53	1.114523	16.869	0.3969	0.6650
0.06	3.49	1.133166	16.988	0.3974	0.6364
0.07	3.47	1.139153	17.039	0.3936	0.5627
0.08	3.43	1.134959	17.181	0.3913	0.5387
0.09	3.42	1.192092	17.415	0.3907	0.5746
0.10	3.30	1.218686	17.637	0.3815	0.5666
At 318.15 K					
0.00	3.78	-	16.247	0.4143	-
0.01	3.66	1.044188	16.556	0.4076	0.7377
0.02	3.62	1.060869	16.656	0.4054	0.8624
0.03	3.59	1.074205	16.746	0.4037	0.6961
0.04	3.53	1.098751	16.884	0.4003	0.7065
0.05	3.48	1.123885	17.025	0.3975	0.7126
0.06	3.45	1.138871	17.130	0.3958	0.6554
0.07	3.41	1.154542	17.242	0.3935	0.6148
0.08	3.35	1.186535	17.432	0.3900	0.6452
0.09	3.27	1.222864	17.676	0.3853	0.6689
0.10	3.21	1.255418	17.896	0.3818	0.6758

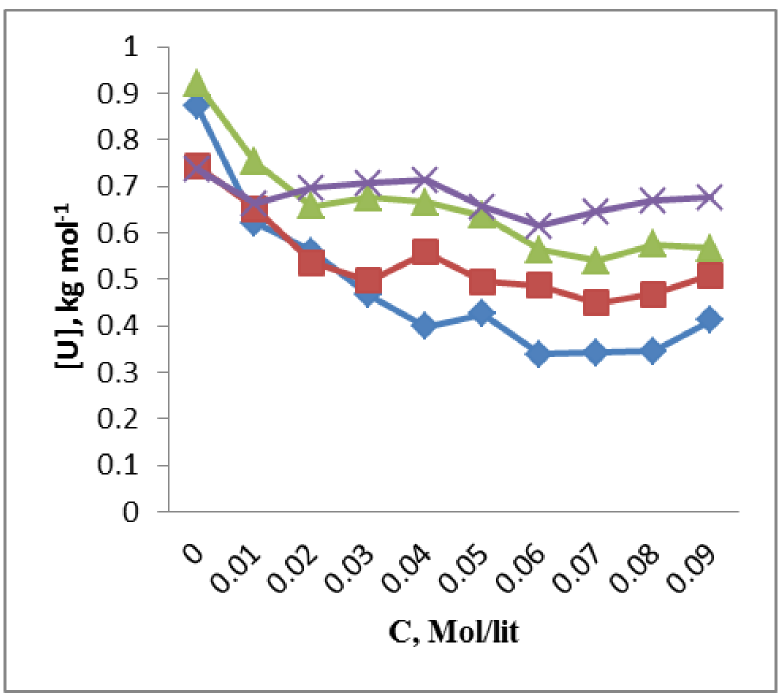

FIG. 5. **Accoustical velocity number [U] plotted against concentration of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution at temperatures 303.15 K (♦), 308.15 K (■), 313.15 K (▲), 318.15 K (×).**

Conclusion

The ultrasonic method is a powerful tool for characterizing physicochemical properties and existence of molecular interaction in a metal – ligand solution. The result reveals that the density and ultrasonic velocity of 2-amino-5-nitrothiazole-$NiCl_2$ aqueous solution increases with increase in concentration and temperature. It is also seen that the formation of a linear, between respective parameters indicated that the stronger solute- solvent interaction and metal –ligand interaction. These results clearly indicate scope for further studies on solute– solvent interaction and metal-ligand interaction and effects of temperature and concentration. These results also give the scope for investigating acoustical parameters of various substituted thiazoles as a ligand with aqueous metal solution.

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