Thakare & Naik, *Cogent Chemistry* (2016), 2: 1242368
http://dx.doi.org/10.1080/23312009.2016.1242368

cogent chemistry

PHYSICAL CHEMISTRY | RESEARCH ARTICLE

Study of molecular interactions of 2-amino-5-nitrothiazole in NNDMF, acetonitrile, and ethanol using acoustical parameters

A.R. Thakare[1,2]* and A.B. Naik[1]

Received: 14 March 2016
Accepted: 22 September 2016
First Published: 29 September 2016

*Corresponding author: A.R. Thakare, Shankarlal Agrawal Science College, Salekasa, Gondia 441916, India
E-mail: avinashrthakare@yahoo.com

Reviewing editor:
Mark Russell St John Foreman, Chalmers University of Technology, Sweden

Additional information is available at the end of the article

Abstract: Density, ultrasonic velocity of binary mixture of 2-amino-5-nitrothiazole + N,N-dimethylformamide (NNDMF), 2-amino-5-nitrothiazole + acetonitrile, and 2-amino-5-nitrothiazole + ethanol were measured at different concentrations of 2-amino-5-nitrothiazole and at different temperatures (303.15, 308.15, 313.15, 318.15 and 323.15) K. Acoustical parameters such as adiabatic compressibility, intermolecular free length, acoustical impedance, sound velocity number, and relative association were determined from experimental data of density and ultrasonic velocity. The effect of temperature and concentration variations in the strength of molecular interaction has been studied. Effective correlation was observed in terms of solute–solvent and solvent–solvent interaction at all temperatures and concentration.

Subjects: Chemistry; Material Science; Materials Science; Physics

Keywords: density; ultrasonic velocity; acoustical parameter; molecular interaction; 2-amino-5-nitrothiazole; NNDMF; acetonitrile and ethanol

1. Introduction

Thiazole and its derivatives are of biological significance (Carbone et al., 2013; Gupta & Kant, 2013; Jalhan, Jindhal, & Gupta, 2012; Saundaneanand, Walmik, Kirankumar, & Annapurna, 2014; Shah, 2014)

ABOUT THE AUTHORS

Our group is made up of four members, out of which two members synthesizes new organic compounds and remaining two peoples studied the physical parameters and biological parameters so as to know details about drug action. Today, mostly used drugs are allopathic drugs which have some harmful effects on the body, but our motto is to prepare and study such drugs, which have less toxic effect, cheaper in cost, and production should be environmentally benign.

PUBLIC INTEREST STATEMENT

In our paper that is, study of molecular interaction of 2-amino-5-nitrothiazole in NNDMF, Acetonitrile, and ethanol using acoustical parameters, the ligand 2-amino-5-nitrothiazole use is an important class of drugs in the therapeutic chemistry and also contributed to the society from biological and industrial point which helps to understand life processes. The knowledge of densities, ultrasonic velocities, and various acoustical parameters are useful for the studies of physicochemical properties of a system. Study of molecular interaction in liquid provides valuable information regarding internal structure molecular association, complex formation, internal pressure etc. The studies of solution properties of liquid solution of polar as well as non polar components have great application in industrial and technological process.

Our group synthesizes new organic compounds and then tries to understand their physicochemical importance so that it will be beneficial for the society.

and the study of molecular interaction in the solution is useful to understand their biological applications. Recently, Otutu, Osabohien, and Efurhievwe (2011) synthesized and studied the spectral properties of hetaryl monoazo dye which is a derivative of 2-amino-5-nitrothiazole. Sulfur- and nitrogen-containing heterocyclic compounds represent an important class of drugs in the therapeutic chemistry and also contributed to the society from biological and industrial point which helps to understand life processes (Shah, 2012). The knowledge of densities, ultrasonic velocities, and various acoustical parameters are useful for the studies of physicochemical properties of a system. Study of molecular interaction in liquid provides valuable information regarding internal structure molecular association, complex formation, internal pressure etc. The studies of solution properties of liquid solution of polar and non-polar components have great applications in industrial and technological process (Talegaonkar, Burghate, & Wadal, 2013). The recent publications (Chauhan, Kumar, & Patial, 2013; Pradhan & Roy, 2014; Singh, Shakya, Shakya, & Yadav, 2012; Stepanov & Minchenko, 2014; Xie, Dong, Zhang, Lu, & Ji, 2014) in this area shows that the many researchers give attention toward study of ultrasonic velocity measurement and study of acoustical properties.

Different liquids flow with different rates depending upon the nature of molecules present in the substance and how easily they slide over one another during their flow. Nagargun, Rao, and Rambabu (2013) have studied speeds of sound and density for binary mixtures of ethyl benzoate (EB) with N,N-dimethylformamide (NNDMF), N,N-dimethylacetamide (NNDMAc), and N,N-dimethylaniline (NNDMA) as a function of mole fraction at different temperature and atmospheric pressure. Recently, Naik, Narwade, Bodakhe, and Muley (2014) reported the molecular interactions in substituted pyrimidines-acetonitrile solutions at different temperature. Measurement of ultrasonic study of an organic ligands solutions provide an excellent method of obtaining data on the ion solvent and solvent–solvent interaction and structure breaking and making properties of solutes. The ultrasonic velocities, densities, and relative association of 2-amino-5-nitrothiazole used in this investigation in polar aprotic–polar protic mixed media at different temperature was lacking and therefore in the present work, we investigate sound velocities and densities for (2-amino-5-nitrothiazole + NNDMF), (2-amino-5-nitrothiazole + acetonitrile), and (2-amino-5-nitrothiazole + ethanol) of different concentrations at temperatures 303.15, 308.15, 313.15, 318.15, and 323.15 K in order to know the effect of temperatures on various acoustical properties. The applications of 2-amino-5-nitrothiazole in different fields of science developed our interest in the measurement of their velocities and densities, and computes the acoustical properties to understand their interaction with non aqueous solvents mixture at different temperature.

2. Materials and experimental

The solvents N,N-dimethylformamide (NNDMF) (Fine-lab, minimum wt. 98%), acetonitrile (Sigma-Aldrich minimum wt. 99%), and ethanol (Sigma-Aldrich minimum wt. 99%) of analytical grade used without purification. The ligand 2-amino-5-nitrothiazole (Hi-MEDIA, minimum wt. 97%) used are of synthesis grade. The ligand solutions in different solvents were prepared by dissolving an accurate amount in an organic solvent in standard flask with airtight caps, and the mass measurements were performed using high-precision digital balance (Adair Datta of accuracy ±0.01 mg). The ultrasonic velocities of pure component and their mixtures were measured by ultrasonic interferometer (Mittal enterprises, model F-81s) at 2 MHz having accuracy ±1 m s^{-1} in velocity. It consists of high-frequency generator and a measuring cell. The densities of NNDMF, acetonitrile, ethanol, and ligand solutions were measured by 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.

3. 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:

$$u = \nu\lambda$$

where u is ultrasonic velocity and λ is wavelength.

The isentropic compressibility β_s was calculated from following equation:

$$\beta_s = 1/\rho u^2$$

where ρ is density of solution and u is speed of ultrasonic velocity.

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

$$L_f = K\beta_s^{1/2}$$

where K is temperature-dependent constant known as a Jacobson constant (Syal, Patial, & Chouhan, 1999).

The acoustic impedance Z is obtained by equation

$$Z = u\rho$$

The relative association R_A was calculated by the following equation:

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

where ρ_o is density of solvent and u_o is velocity of solvent. Also, the sound velocity number is calculated from following equation:

$$[U] = u - u_o/u_o c$$

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

4. Results and discussion

The calibration of the ultrasonic interferometer was done by measuring the ultrasonic velocities and densities of the pure NNDMF, acetonitrile, and ethanol, respectively. The measured value is found to be in good concordance with literature values which are shown in Table 1. Small difference may occur due to difference in purity of chemicals, measurements, techniques, and calibrations.

The values of densities and ultrasonic velocities for systems 2-amino-5-nitrothiazole + NNDMF, 2-amino-5-nitrothiazole + acetonitrile, and 2-amino-5-nitrothiazole + ethanol respectively are listed in Table 2 and the values of acoustical parameters such as adiabatic compressibility, relative association, acoustical impedance, linear free length, and sound velocity number are listed in Tables 3–5, respectively. In this investigation, the value of density and ultrasonic velocity increases with increase in the concentration of 2-amino-5-nitrothiazole and decreases with increase in the temperature at any particular concentration for all the three systems (Figures 1–5). The values from Table 2 show that ultrasonic velocity values decrease with increase in temperature due to the breakage of hetero- and homomolecular clusters at high temperatures (Nagargun et al., 2013). The decrease in ultrasonic velocity and density with increase in temperature indicates that cohesive forces decreased (Godhani, Dobariya, Sanghani, & Mehta, 2012). The increasing temperature has two opposite effects namely increase in molecular interaction (structure formation) and destruction of structure formed previously. When the thermal energy is greater than the interaction energy, it causes the destruction of previously formed structure. Thus, the increase in temperature favors the increase in kinetic energy and volume expansion and hence, results in the decrease in ρ and u. Also, these results indicate that there is a significant interaction between the solute and solvent molecules because the presence of amine group of 2-amino-5-nitrothiazole and alcoholic group of ethanol creates the possibility of hydrogen bonding between molecules.

Table 1. Experimental and literature values of density and ultrasonic velocity, respectively

	T (K)	Expt		Lit	
		u_0 (ms^{-1})	ρ_0 (kg m^{-3})	u_0 (ms^{-1})	ρ_0 (kg m^{-3})
NNDMF	303.15	1458	0.9531	1456 (Syal, Patial, & Chouhan, 1999)	–
	308.15	1432	0.9386	1424 (Attri, Reddy, & Venkatesu, 2010)	0.934 (Attri et al., 2010)
	318.15	1389	0.9303	1386 (Attri et al., 2010)	0.925 (Attri et al., 2010)
Acetonitrile	303.15	1276	0.7724	1278 (Grande, Juliá, Barrero, & Marschoff, 2013)	0.771 (Grande et al., 2013)
	308.15	1240	0.7669	1239 (Grande et al., 2013)	0.765 (Grande et al., 2013)
	313.15	1216	0.7591	1218 (Grande et al., 2013)	0.760 (Grande et al., 2013)
	318.15	1198	0.7522	1198 (Grande et al., 2013)	0.754 (Grande et al., 2013)
	323.15	1174	0.7491	1177 (Grande et al., 2013)	0.749 (Grande et al., 2013)
Ethanol	303.15	1134	0.7786	1131 (Naidu & Prasad, 2004)	0.779 (Naidu & Prasad, 2004)
	308.15	1116	0.7758	1115 (Naidu & Prasad, 2004)	0.776 (Aminabhavi & Banerjee, 1998)
	313.15	1096	0.7722	1099 (Naidu & Prasad, 2004)	0.773 (Naidu & Prasad, 2004)
	318.15	1074	0.7687	1075 (Gong, Shen, Lu, Meng, & Li, 2012)	0.768 (Pandey, Awasthi, & Awasthi, 2014)
	323.15	1062	0.7643	1066 (Naidu & Prasad, 2004)	0.765 (Naidu & Prasad, 2004)

Note: Uncertainties in temperature, density and velocity are 0.1 K, 1 m s^{-1} and 0.0005 kg m^{-3}.

When there is an ultrasonic wave 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 (Godhani et al., 2012). 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 increase in isentropic compressibility (β) with increase in temperature might be due to molecular interaction in solution which supports solvent-solute interactions. Figures 6–8 it clearly indicate that the isentropic compressibility increases with increase in temperature and decreases with increase in concentration of solute. The decrease in isentropic compressibility with increasing concentration of 2-amino-5-nitrothiazole clearly indicates the presence of solute–solvent interactions due to aggregation of solvent molecules around solute molecules (Thirumaran & Rajeswari, 2011). The variation in ultrasonic velocity in a solution depends on the intermolecular free length on mixing. On the basis of a model for sound propagation given by Kincaid and Eyring (1938), ultrasonic velocity increases with decrease in free length (L_f) and vice versa. Intermolecular free length is a predominant factor for determining the variation in ultrasonic velocity, in liquids and their solutions (Landge, Badade, & Kendre, 2013). Intermolecular free length (L_F) is the distance between the surfaces of the neighboring molecules and indicates a significant interaction between solute–solvent and solvent–solvent molecules (Yadav, Kumar, & Yadav, 2014). From graph, we say that increase in U and decrease in Lf indicate close association between solute and solvent molecules, whereas reverse of these suggest solute–solute interactions. Hence, it is also a good tool to investigate the molecular interactions in the binary solvent mixture. 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 ion (Kharkale, Bhaskar, Agarwal, & Paliwal, 2013); it means ions restricts free flow of sound wave. The character that decreases this restriction or backward movement of sound waves is known as acoustic impedance (Z). From Figures 9–11 it is clearly observed that the value of acoustic impedance decreases as temperature increases. If the temperature increases, ultrasonic velocity decreases and value of

Table 2. Experimental values of density and ultrasonic velocity of 2-amino-5-nitrothiazole + NNDMF, 2-amino-5-nitrothiazole + acetonitrile and 2-amino-5-nitrothiazole + ethanol at different concentrations and at different 303.15, 308.15, 313.15, 318.15, and 323.15 K respectively

C (mol/l)	ρ (g cm^{-3})					*u* (m s^{-1})				
	303.15	308.15	313.15	318.15	323.15	303.2	308.15	313.15	318.15	323.15
NNDMF + 2-amino-5-nitrothiazole										
0.00	0.9531	0.9382	0.9307	0.9241	0.9193	1458	1432	1402	1389	1364
0.01	0.9636	0.9438	0.9365	0.9328	0.9239	1468	1438	1406	1397	1372
0.02	0.9755	0.9476	0.9418	0.9373	0.9286	1472	1442	1416	1408	1392
0.03	0.9832	0.9494	0.9432	0.9414	0.9360	1464	1450	1410	1416	1398
0.04	0.9898	0.9533	0.9498	0.9466	0.9437	1478	1456	1418	1420	1409
0.05	0.9975	0.9647	0.9569	0.9532	0.9484	1486	1448	1438	1431	1416
0.06	1.0046	0.9715	0.9643	0.9617	0.9562	1494	1452	1444	1438	1428
0.07	1.0194	0.9842	0.9757	0.9692	0.9635	1490	1464	1458	1446	1436
0.08	1.0273	1.0029	0.9834	0.9786	0.9720	1502	1466	1450	1452	1444
0.09	1.0366	1.0174	0.9985	0.9831	0.9802	1505	1462	1554	1456	1450
0.10	1.0447	1.0251	1.0122	0.9960	0.9911	1509	1478	1462	1460	1456
Acetonitrile + 2-amino-5-nitrothiazole										
0.00	0.7721	0.7663	0.7592	0.7527	0.7490	1276	1240	1216	1198	1216
0.01	0.7755	0.7691	0.7633	0.7578	0.7531	1278	1246	1220	1204	1220
0.02	0.7802	0.7747	0.7685	0.7629	0.7585	1286	1252	1226	1210	1226
0.03	0.7860	0.7765	0.7721	0.7656	0.7615	1290	1260	1236	1222	1236
0.04	0.7882	0.7810	0.7762	0.7713	0.7682	1296	1262	1244	1232	1244
0.05	0.7962	0.7874	0.7816	0.7787	0.7738	1304	1268	1252	1244	1252
0.06	0.7998	0.7936	0.7887	0.7874	0.7792	1306	1264	1258	1250	1258
0.07	0.8052	0.7981	0.7939	0.7915	0.7867	1302	1272	1254	1258	1254
0.08	0.8116	0.8028	0.7968	0.7950	0.7900	1310	1284	1266	1268	1266
0.09	0.8164	0.8125	0.7991	0.7985	0.7943	1324	1294	1280	1274	1280
0.10	0.8216	0.8173	0.8087	0.8022	0.7997	1336	1302	1296	1288	1296
Ethanol + 2-amino-5-nitrothiazole										
0.00	0.7781	0.7757	0.7723	0.7682	0.7641	1134	1116	1096	1074	1062
0.01	0.7793	0.7788	0.7765	0.7715	0.7683	1136	1122	1098	1078	1068
0.02	0.7845	0.7821	0.7792	0.7762	0.7748	1138	1126	1106	1084	1074
0.03	0.7912	0.7892	0.7851	0.7813	0.7792	1146	1134	1114	1088	1072
0.04	0.7942	0.7936	0.7895	0.7864	0.7834	1152	1130	1124	1096	1080
0.05	0.7993	0.7965	0.7947	0.7892	0.7900	1164	1146	1132	1106	1090
0.06	0.8075	0.7991	0.7899	0.7878	0.7934	1178	1158	1144	1114	1094
0.07	0.8164	0.8082	0.8305	0.7947	0.7917	1192	1166	1158	1122	1102
0.08	0.8216	0.8182	0.8095	0.7996	0.7975	1198	1172	1164	1136	1116
0.09	0.8323	0.8251	0.8161	0.8075	0.8055	1206	1188	1176	1142	1128
0.10	0.8427	0.8372	0.8280	0.8181	0.8148	1218	1196	1188	1156	1142

Note: Uncertainties in temperature, density and velocity are 0.1 K, 1 m s^{-1} and 0.001 kg m^{-3}.

Table 3. Isentropic compressibility, relative association, acoustic impedance, linear length and sound velocity number for 2-amino-5-nitrothiazole + NNDMF at different temperature and different concentration

C (mol/l)	$\beta_s \times 10^{-10}$ (m² N⁻¹)	R_A	$Z \times 10^{-5}$ (kg m² s⁻¹)	L_f (A⁰)	[*U*] (kg mol⁻¹)
303.15 K					
0.00	4.93	–	13.894	0.4608	–
0.01	4.79	1.0241	14.210	0.4542	0.6858
0.02	4.73	1.0539	14.352	0.4514	0.4801
0.03	4.74	1.0742	14.391	0.4518	0.4371
0.04	4.62	1.0904	14.617	0.4461	0.3429
0.05	4.54	1.1241	14.815	0.4422	0.3840
0.06	4.46	1.1501	14.999	0.4383	0.4115
0.07	4.42	1.1530	15.183	0.4363	0.3135
0.08	4.31	1.2073	15.425	0.4308	0.3772
0.09	4.26	1.2363	15.591	0.4283	0.3581
0.10	4.20	1.2639	15.753	0.4253	0.3497
308.15 K					
0.00	5.19	–	13.432	0.4771	–
0.01	5.12	1.0266	13.560	0.4738	0.4189
0.02	5.07	1.0780	13.655	0.4715	0.4391
0.03	5.01	1.0966	13.760	0.4687	0.4189
0.04	4.94	1.1287	13.875	0.4654	0.4416
0.05	4.94	1.1540	13.958	0.4654	0.2230
0.06	4.88	1.1936	14.098	0.4626	0.2327
0.07	4.74	1.2239	14.405	0.4559	0.3192
0.08	4.64	1.2531	14.689	0.4511	0.2967
0.09	4.60	1.2783	14.868	0.4491	0.2327
0.10	4.27	1.3111	15.149	0.4327	0.3212
313.15 K					
0.00	5.47	–	13.038	0.4942	–
0.01	5.40	1.0195	13.160	0.4910	0.2853
0.02	5.30	1.0400	13.324	0.4864	0.4992
0.03	5.33	1.0810	13.296	0.4878	0.1902
0.04	5.24	1.1159	13.456	0.4837	0.2853
0.05	5.05	1.1550	13.747	0.4748	0.5135
0.06	4.97	1.1860	13.920	0.4710	0.4992
0.07	4.82	1.2132	14.213	0.4633	0.5706
0.08	4.83	1.2540	14.253	0.4643	0.4279
0.09	4.73	1.3310	14.510	0.4641	0.4121
0.10	4.62	1.3401	14.795	0.4541	0.4279

(*Continued*)

Table 3. (*Continued*)

C (mol/l)	$\beta_s \times 10^{-10}$ (m^2 N^{-1})	R_A	$Z \times 10^{-5}$ (kg m^2 s^{-1})	L_f (A^0)	[*U*] (kg mol^{-1})
318.15 K					
0.00	5.60	–	12.834	0.5044	–
0.01	5.49	1.0249	13.022	0.4994	0.5722
0.02	5.38	1.0394	13.192	0.4944	0.6839
0.03	5.30	1.0650	13.324	0.4907	0.6479
0.04	5.24	1.1061	13.433	0.4884	0.5579
0.05	5.12	1.1554	13.637	0.4823	0.6047
0.06	5.03	1.2213	13.819	0.4781	0.5879
0.07	4.93	1.2515	14.011	0.4733	0.5862
0.08	4.84	1.3007	14.200	0.4689	0.5669
0.09	4.79	1.3123	14.312	0.4665	0.5359
0.10	4.71	1.3694	14.541	0.4626	0.5111
323.15 K					
0.00	5.84	–	12.535	0.5197	–
0.01	5.75	1.0155	12.663	0.5156	0.5865
0.02	5.56	1.0448	12.917	0.5070	0.5026
0.03	5.46	1.0563	13.085	0.5025	0.8308
0.04	5.34	1.0896	13.286	0.4969	0.8047
0.05	5.26	1.1272	13.423	0.4932	0.7624
0.06	5.12	1.1609	13.651	0.4866	0.7820
0.07	5.03	1.1964	13.828	0.4823	0.7540
0.08	4.93	1.2473	14.035	0.4775	0.7331
0.09	4.85	1.2745	14.210	0.4736	0.7005
0.10	4.75	1.3304	14.428	0.4687	0.6744

Table 4. Isentropic compressibility, relative association, acoustic impedance, linear length and sound velocity number for 2-amino-5-nitrothiazole + acetonitrile at different temperature and different concentration

C (mol/lit)	$\beta_s \times 10^{-10}$ (m^2 N^{-1})	R_A	$Z \times 10^{-5}$ (kg m^2 s^{-1})	L_f (A^0)	[*U*] (kg mol^{-1})
303.15 K					
0.00	7.95	–	9.850	0.5852	–
0.01	7.90	1.0212	9.904	0.5833	0.5167
0.02	7.75	1.0451	10.03	0.5778	0.3918
0.03	7.65	1.0461	10.13	0.5740	0.3657
0.04	7.55	1.0764	10.21	0.5703	0.3918
0.05	7.38	1.1107	10.37	0.5638	0.4388
0.06	7.33	1.1203	10.43	0.5619	0.3918
0.07	7.32	1.1550	10.48	0.5615	0.2910
0.08	7.18	1.2072	10.62	0.5561	0.3330
0.09	6.99	1.2593	10.80	0.5487	0.4179
0.10	6.82	1.3253	10.93	0.5420	0.4702
308.15 K					
0.00	8.49	–	9.498	0.6102	–
0.01	8.32	1.0264	9.581	0.6066	0.4838

(*Continued*)

Table 4. (*Continued*)

C (mol/lit)	$\beta_s \times 10^{-10}$ (m² N⁻¹)	R_A	$Z \times 10^{-5}$ (kg m² s⁻¹)	L_f (A⁰)	[*U*] (kg mol⁻¹)
0.02	8.22	1.0440	9.690	0.6004	0.4838
0.03	8.11	1.0344	9.777	0.5964	0.5376
0.04	8.03	1.0682	9.856	0.5934	0.4435
0.05	7.99	1.0910	9.979	0.5919	0.4516
0.06	7.89	1.1188	10.02	0.5882	0.3225
0.07	7.74	1.1064	10.15	0.5826	0.3686
0.08	7.56	1.1427	10.29	0.5758	0.4435
0.09	7.35	1.1609	10.50	0.5677	0.4838
0.10	7.22	1.1814	10.63	0.5627	0.5001
313.15 K					
0.00	8.91	–	9.229	0.6307	–
0.01	8.85	1.0303	9.308	0.6286	0.3289
0.02	8.66	1.0212	9.415	0.6218	0.4111
0.03	8.47	1.0785	9.541	0.6149	0.5482
0.04	8.32	1.0917	9.653	0.6095	0.5756
0.05	8.16	1.0845	9.778	0.6036	0.5921
0.06	8.01	1.0984	9.913	0.598	0.5756
0.07	8.01	0.1427	9.944	0.598	0.4464
0.08	7.83	1.1585	10.077	0.5912	0.5139
0.09	7.63	1.1584	10.227	0.5836	0.5847
0.10	7.36	1.1024	10.471	0.5732	0.6578
318.15 K					
0	9.26	–	9.008	0.6487	–
0.01	9.11	1.0140	9.114	0.6434	0.5008
0.02	8.96	1.0398	9.220	0.6381	0.5069
0.03	8.75	1.0294	9.348	0.6305	0.6677
0.04	8.54	1.0524	9.498	0.6229	0.7095
0.05	8.30	1.0822	9.678	0.6141	0.7679
0.06	8.13	1.1340	9.837	0.6441	0.7234
0.07	7.98	1.1819	9.950	0.6022	0.7154
0.08	7.82	1.1847	10.08	0.5961	0.7303
0.09	7.72	1.2100	10.16	0.5923	0.7048
0.1	7.51	1.2420	10.32	0.5842	0.7525
323.15 K					
0.00	9.68	–	8.793	0.6690	–
0.01	9.53	1.0090	8.885	0.6638	0.5110
0.02	9.41	1.0340	8.974	0.6597	0.4258
0.03	9.24	1.0523	9.071	0.6537	0.5110
0.04	8.98	1.0705	9.246	0.6444	0.6388
0.05	8.72	1.1021	9.415	0.6350	0.7495
0.06	8.40	1.1087	9.628	0.6232	0.8801
0.07	8.22	1.1071	9.777	0.6165	0.8517
0.08	7.99	1.1363	9.938	0.6078	0.8943
0.09	7.90	1.1824	10.02	0.6044	0.8328
0.10	7.68	1.2204	10.19	0.5959	0.8688

cogent • chemistry

Table 5. Isentropic compressibility, relative association, acoustic impedance, linear length and sound velocity number for 2-amino-5-nitrothiazole + acetonitrile at different temperature and different concentrations

C (mol/l)	$\beta_s \times 10^{-10}$ (m^2 N^{-1})	R_A	$Z \times 10^{-5}$ (kg m^2 s^{-1})	L_f (A^0)	[*U*] (kg mol^{-1})
303.15 K					
0.00	9.99	–	8.8225	0.5602	–
0.01	9.94	1.0181	8.8494	0.6543	0.1763
0.02	9.84	1.0409	8.9219	0.6510	0.1763
0.03	9.62	1.0632	9.0648	0.6437	0.3527
0.04	9.49	1.0760	9.1468	0.6393	0.3968
0.05	9.23	1.1012	9.3060	0.6305	0.5291
0.06	8.92	1.0963	9.7420	0.6198	0.6466
0.07	8.62	1.1266	9.7267	0.6093	0.7306
0.08	8.48	1.1639	9.8355	0.6044	0.7054
0.09	8.26	1.2056	10.033	0.5965	0.7045
0.10	8.05	1.2355	10.255	0.5888	0.7407
308.15 K					
0.00	10.3	–	8.649	0.6721	–
0.01	10.2	1.0152	8.729	0.6688	0.5376
0.02	10.0	1.0371	8.805	0.6649	0.4480
0.03	9.85	1.0681	8.947	0.6572	0.5376
0.04	9.87	1.0948	8.96	0.6579	0.3136
0.05	9.56	1.1231	9.122	0.6475	0.5376
0.06	9.33	1.1495	9.252	0.6397	0.6272
0.07	9.10	1.1460	9.421	0.6317	0.6400
0.08	8.82	1.1834	9.586	0.6219	0.6272
0.09	8.58	1.2278	9.801	0.6134	0.7168
0.1	8.35	1.2890	10.01	0.6051	0.7168
313.15 K					
0.00	10.70	–	8.461	0.9912	–
0.01	10.60	1.0231	8.520	0.6879	0.1824
0.02	10.40	1.0186	8.615	0.6814	0.4562
0.03	10.20	1.0494	8.744	0.6748	0.5474
0.04	10.03	1.0533	8.868	0.6692	0.6386
0.05	9.82	1.0110	8.988	0.6621	0.6569
0.06	9.57	1.1627	9.083	0.6536	0.7290
0.07	9.28	1.2182	9.298	0.6437	0.8081
0.08	9.12	1.2448	9.416	0.6381	0.7755
0.09	8.86	1.2867	9.596	0.6289	0.8110
0.10	8.55	1.3410	9.836	0.6178	0.8394
318.15 K					
0.00	11.2	–	8.248	0.7134	–
0.01	11.1	1.0202	8.311	0.7121	0.3724
0.02	10.9	1.0364	8.411	0.7038	0.4655
0.03	10.8	1.0681	8.497	0.7005	0.4345
0.04	10.5	1.0622	8.614	0.6907	0.5121

(*Continued*)

Table 5. (*Continued*)

C (mol/l)	$\beta_s \times 10^{-10}$ ($m^2 N^{-1}$)	R_A	$Z \times 10^{-5}$ (kg $m^2 s^{-1}$)	L_f (A^0)	[*U*] (kg mol^{-1})
0.05	10.4	1.1121	8.726	0.6874	0.5959
0.06	10.2	1.1518	8.767	0.6808	0.6207
0.07	10.0	1.1647	8.908	0.9741	0.6384
0.08	9.69	1.2224	9.076	0.6636	0.7216
0.09	9.50	1.2844	9.215	0.6570	0.7034
0.10	9.14	1.3293	9.456	0.6444	0.7635
323.15 K					
0.00	11.6	–	8.113	0.7324	–
0.01	11.4	1.0108	8.202	0.7261	0.5649
0.02	11.2	1.0370	8.312	0.7197	0.5649
0.03	11.1	1.0678	8.350	0.7164	0.3138
0.04	10.9	1.1026	8.456	0.7100	0.4237
0.05	10.6	1.1334	8.611	0.7001	0.5273
0.06	10.5	1.1755	8.675	0.6968	0.5021
0.07	10.4	1.2270	8.786	0.6935	0.5380
0.08	10.0	1.2556	8.894	0.6824	0.6355
0.09	9.76	1.3059	9.080	0.6718	0.6905
0.10	9.41	1.3661	9.295	0.6597	0.7532

Figure 1. Density (*ρ*) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2- amino-5-nitrothazole + NNDMF (■), 2-amino-5-nitrothiazole + acetonitrile (▲), and 2-amino-5-nitrothiazole + ethanol (×) at 303.15 K.

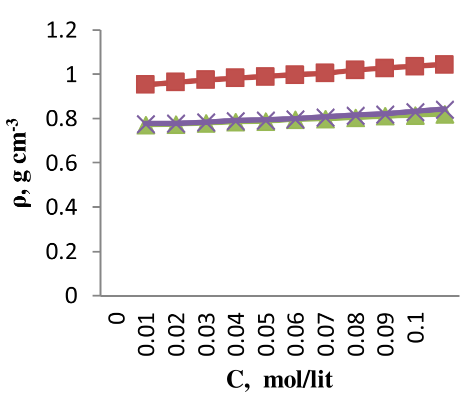


Figure 2. Ultrasonic velocity (*u*) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + NNDMF (■), 2-amino-5-nitrothiazole + acetonitrile (▲), and 2-amino-5-nitrothiazole + ethanol (×) 303.15 K.

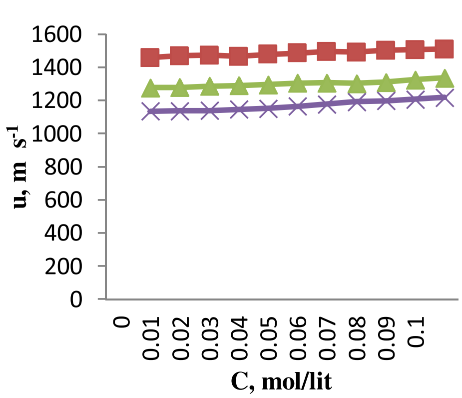


Figure 3. Ultrasonic velocity (*u*) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + NNDMF at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

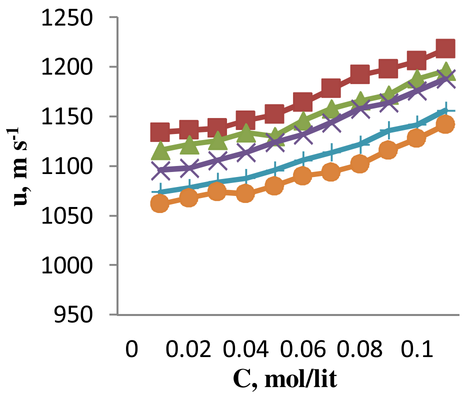


Figure 4. Ultrasonic velocity (*u*) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + Acetonitrile at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

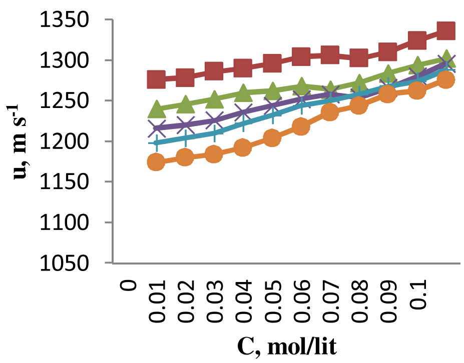
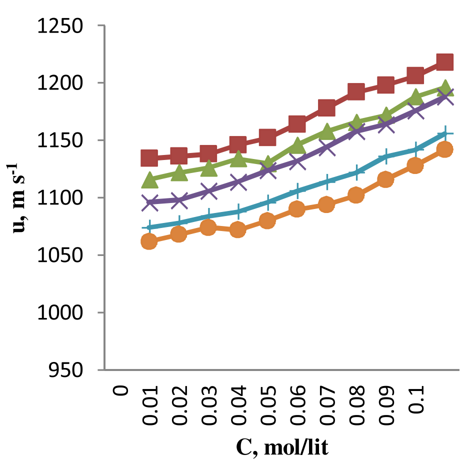


Figure 5. Ultrasonic velocity (*u*) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + Ethanol at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).



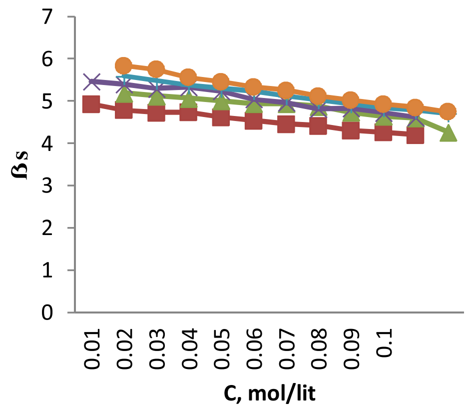


Figure 6. Isentropic compressibility plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + NNDMF at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

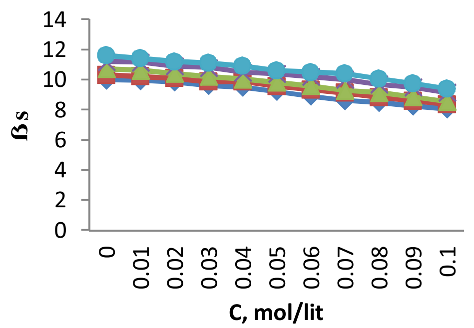


Figure 7. Isentropic compressibility plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + Acetonitrile at temperatures 303.15 K (◆), 308.15 K (■), 313.15 K (▲), 318.15 K (×), and 323.15 K (●).

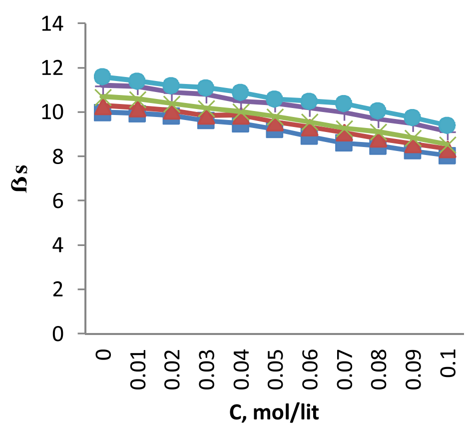


Figure 8. Isentropic compressibility plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + Ethanol at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

Figure 9. Specific acoustic impedance plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + NNDMF at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

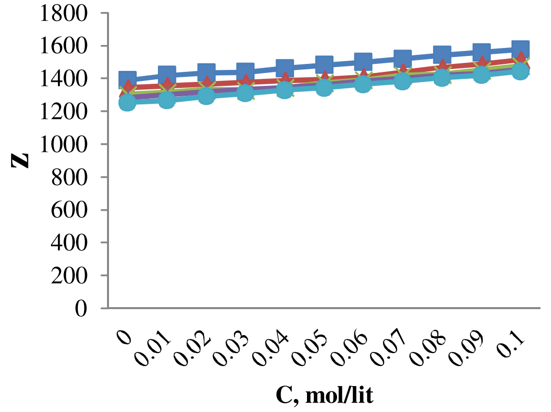


Figure 10. Specific acoustic impedance plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + acetonitrile at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

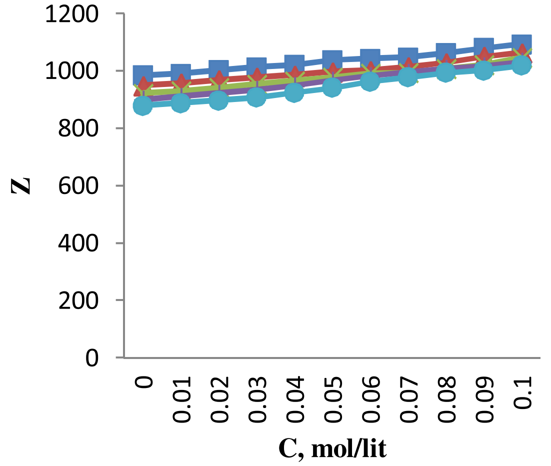


Figure 11. Specific acoustic impedance plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + ethanol at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

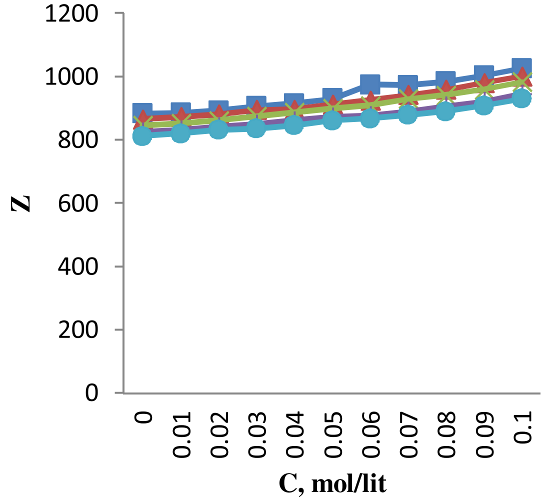


Figure 12. Relative association (R_A) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + NNDMF at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

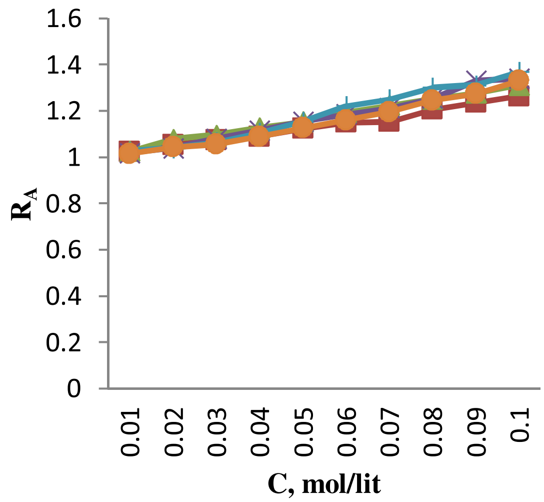


Figure 13. Relative association (R_A) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + acetonitrile at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15 K (●).

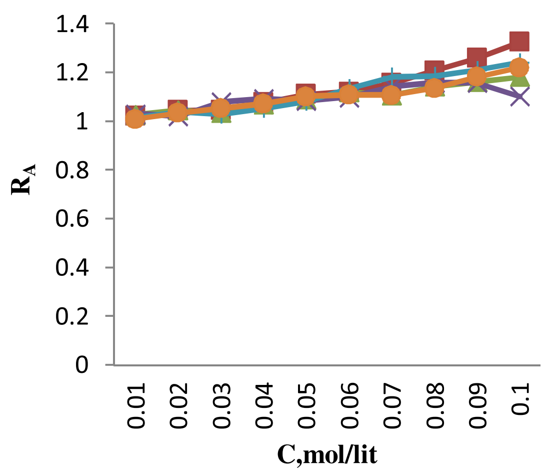
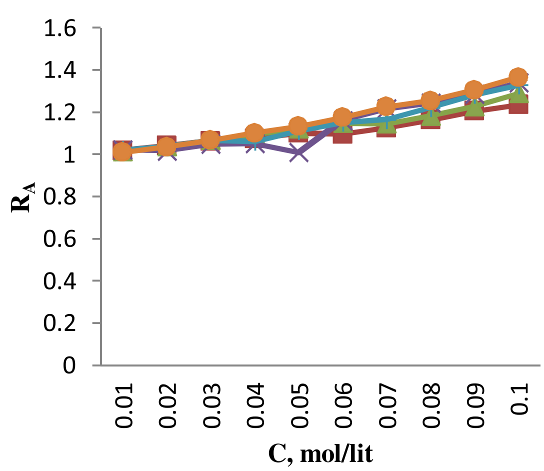


Figure 14. Relative association (R_A) plotted against concentration of 2-amino-5-nitrothiazole in binary mixture of 2-amino-5-nitrothazole + ethanol at temperatures 303.15 K (■), 308.15 K (▲), 313.15 K (×), 318.15 K (+), and 323.15K



acoustic impedance (*Z*) decreases (Landge et al., 2013) as acoustic impedance (*Z*) is the product of ultrasonic velocity (*u*) and density (ρ). Also, in this present investigation, it is observed that these acoustic impedance (*Z*) value increase with increase in concentration of 2-amino-5-nitrothiazole in acetonitrile, ethanol, NNDMF solutions, respectively. The linear variation in acoustic impedance with concentration confirms the presence of molecular association between the solute–solvent molecules. Such an increasing trends of impedance further support the possibility of molecular interaction between the solute–solvent. Figures 12–14 shows that the relative association (R_A) increases with increase in temperature and the increase in concentration of solution. This is due to the solute–solvent interaction that dominates over solvent–solvent 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 (Ambomase, Tripathy, Tripathy, & Dash, 2011; Meshram, Agrawal, Chandak, & Chapke, 2013). In general, sound velocity number increases with increase in concentration of solute (Chauhan et al., 2013) and increase in temperature, however in present investigation, there is no regular variation observed in sound velocity number.

5. Conclusions

The ultrasonic method is a powerful tool for characterizing physicochemical properties and existence of molecular interaction in the mixture. The result reveals that the density and ultrasonic velocity of 2-amino-5-nitrothiazole + NNDMF, 2-amino-5-nitrothiazole + Acetonitrile, and 2-amino-5-nitrothiazole + ethanol solutions decrease with increase in temperature. It is also seen that the formation of linear plot between and respective parameters indicated the stronger solute–solvent interaction.

Funding

This work was financially supported by the Department of Science and Technology [grant number SERB/F/4566/2013–14].

Author details

A.R. Thakare[1,2]

E-mail: avinashrthakare@yahoo.com

A.B. Naik[1]

E-mail: naikabn@gmail.com

[1] Department of Chemical Technology, Sant Gadge Baba Amravati University, Amravati 444602, India.

[2] Shankarlal Agrawal Science College, Salekasa, Gondia 441916, India.

Citation information

Cite this article as: Study of molecular interactions of 2-amino-5-nitrothiazole in NNDMF, acetonitrile, and ethanol using acoustical parameters, A.R. Thakare & A.B. Naik, *Cogent Chemistry* (2016), 2: 1242368.

References

Ambomase, S., Tripathy, S., Tripathy, M., & Dash, U. N. (2011). Studies on water-polymer interactions inthe presence of aceclofenac at 298.15 K. *E-Journal of Chemistry, 8*, 63–70. http://dx.doi.org/10.1155/2011/545313

Aminabhavi, T. M., & Banerjee, K. (1998). Density, viscosity, refractive index, and speed of sound in binary mixtures of 2-chloroethanol with alkanols (C1–C6) at 298.15, 303.15, and 308.15 K. *Journal of Chemical & Engineering Data, 43*, 509–513. http://dx.doi.org/10.1021/je9702596

Attri, P., Reddy, P., & Venkatesu, P. (2010). Drnsity ultrasonic sound speed measurement for NN-dimethylformaide with ionic liquids. *Indian Journal of Pure and Applied Physics, 49*, 736–742.

Carbone, A., Pennati, M., Parrino, B., Lopergolo, A., Barraja, P., Montalbano, A., ... Zaffaroni, N. (2013). Novel 1 H-pyrrolo[2,3- b]pyridine derivative nortopsentin analogues: Synthesis and antitumor activity in peritoneal mesothelioma experimental models. *Journal of Medicinal Chemistry, 56*, 7060–7072. http://dx.doi.org/10.1021/jm400842x

Chauhan, S., Kumar, K., & Patial, B. (2013). Study of acoustic parameters of proline in lecithin-ethanol mixture at varying temperature. *Indian Journal of Pure and Applied Physics, 51*, 531–541.

Godhani, R., Dobariya, B., Sanghani, A., & Mehta, P. (2012). Thermodynamic properties of binary mixtures of 1,3,4-oxadiazole derivative with chloroform, NN-dimethylformamide 303.15-313.15 K and atmospheric pressure. *Arabian Journal of Chemistry*. doi:10.1016/arabjc/2012.10.002.

Gong, Y., Shen, C., Lu, Y., Meng, H., & Li, C. (2012). Viscosity and density measurements for six binary mixtures of water (methanol or ethanol) with an ionic liquid ([BMIM][DMP] or [EMIM][DMP]) at atmospheric pressure in the temperature range of (293.15 to 333.15) K. *Journal of Chemical & Engineering Data, 57*, 33–39. http://dx.doi.org/10.1021/je200600p

Grande, M. D. C., Juliá, J. Á., Barrero, C. R., Marschoff, C. M. (2013). Sound velocity measurements in the water+acetonitrile system at temperatures from 293.15 to 323.15K and its implications on thermodynamic data processing. *Physics and Chemistry of Liquids, 51*, 457–468. http://dx.doi.org/10.1080/00319104.2012.737790

Gupta, V., & Kant, V. (2013). A review on biological activity of imidazole and thiazole moieties and their derivatives. *Science International, 1*, 253–260. http://dx.doi.org/10.17311/sciintl.2013.253.260

Jalhan, S., Jindhal, A., & Gupta, A. (2012). Synthesis, biological activities and chemistry of thiadiazoles and Schiff bases. *Asian Journal of Pharmaceutical and Clinical Research, 5*, 199–208.

Kharkale, S., Bhaskar, C., Agarwal, P., & Paliwal, P. (2013). A study of substituded dihydroformazan in predicting the acoustical and its allied properties in different solvents at 288.15 K. *International Journal of Emerging Technologies in Computational and Applied Sciences, 5*, 327–329.

Kincaid, J., & Eyring, H. (1938). The liquid state. *The Journal of Chemical Physics, 6*, 587–620.

Landge, M., Badade, S., & Kendre, B. (2013). Density, ultrasonic velocity and viscosity measurements of gluc glucose-alcohol-water mixtures at various temperatures. *International Journal of Research in Chemistry and Environment, 3*, 348–352.
Meshram, B., Agrawal, P., Chandak, H., & Chapke, U. (2013). A study of acoustical behaviour of paracetamol in 70% methanol at various temperature. *International Journal of Emerging Technologies in Computational and Applied Sciences, 5*, 369–373.
Nagargun, B., Rao, G., & Rambabu, C. (2013). Thermodynamic and acoustic study on molecular interactions in certain binary liquid systems involving ethyl benzoate. *Journal of Thermodynamics*. doi:10.1155/2013/285796
Naidu, P., & Prasad, K. (2004). Ultrasonic velocity and allied parameters in solutions of cypermethrin with xylene and ethanol. *Indian Journal of Pure and Applied Physics, 42*, 512–517.
Naik, A., Narwade, M. L., Bodakhe, P., & Muley, G. (2014). Molecular interactions in substituted pyrimidines-acetonitrile solutions at 298.15–318.15 K. *Russian Journal of Physical Chemistry A, 88*, 37–41. http://dx.doi.org/10.1134/S0036024414010324
Otutu, J., Osabohien, E., & Efurhievwe, E. (2011). Synthesis and spectral properties of hetaryl monoazo dyes derived from 2-amino-5-nitrothiazole. *Oriental Journal of Chemistry, 27*, 1389–1396.
Pandey, P., Awasthi, A., & Awasthi, A. (2014). Intermolecular interactions in ternary system of 2-dimethylaminoethanol + methanol + ethanol at various temperatures: Ultrasonic, volumetric and IR study. *Physics and Chemistry of Liquids, 52*, 416–427. http://dx.doi.org/10.1080/00319104.2013.852478
Pradhan, P., & Roy, M. (2014). Studies on solution properties of ternary mixture of acetophenone + n -amyl alcohol + dichloromethane and its corresponding binaries at 298.15 K. *Physics and Chemistry of Liquids, 52*, 100–112. http://dx.doi.org/10.1080/00319104.2011.604779
Saundaneanand, R., Walmik, P., Kirankumar, M., & Annapurna, H. (2014). Synthesis of novel N-(Aryl) diazolyl thiazol-2-amines and benzylidene-thiazolidin-4-ones linked to indole nucleus as antioxidant, antimicrobial, antimicrobacterial, and cytotoxic agents. *International Journal of Pharmacy and Pharmaceutical Sciences, 6*, 141–147.
Shah, P. (2012). Synthesis and biological activity of novel imidazole. *Current Trends in Biotechnology and Chemical Research, 2*, 45–51.
Shah, P. (2014). Studies of novel thiazole-imidazole combined molecule. *Octa. Journal of Environmental Research, 2*, 48–52.
Singh, I., Shakya, N., Shakya, N., Yadav, S. (2012). Investigation of type of interaction between salicylic acid and ethanol at different temperatures. *International Journal of Chemical, Environmental and Pharmaceutical Research, 3*, 127–129.
Stepanov, V., & Minchenko, V. (2014). Sound Velocities for Dissolving AgI + LiCl Melts. *Journal of Chemical & Engineering Data, 59*, 3888–3893 doi:10.1021/je500781j
Syal, V., Patial, B., & Chouhan, S. (1999). Ultrasonic velocity, viscocity and density dtudies in binary mixture of dimethylformaide and ethyl methyl ketone at different temperatures. *Indian Journal of Pure and Applied Physics, 37*, 366–370.
Talegaonkar, R., Burghate, A., & Wadal, A. (2013). Acoustical properties of substituted thiazolyl schiff`s base in binary solvent mixture at fixed temperature. *Rasayan Journal of Chemistry, 6*, 7–11.
Thirumaran, S., & Rajeswari, M. (2011). Acoustical study on binary liquid mixture of some aromatic hydrocarbons with DMSO at 303.15 K. *Scholars Research Library, 2*, 149–156.
Xie, Y., Dong, H., Zhang, S., Lu, X., & Ji, X. (2014). Effect of water on the density, viscosity, and CO_2 Solubility in choline chloride/urea. *Journal of Chemical & Engineering Data, 59*, 3344–3352. doi:10.1021/je500320c
Yadav, P., Kumar, M., & Yadav, R. (2014). Study of molecular interaction in binary liquid mixtures of ethyl acetoacetate with chloroform and dimethylsulphoxide using excess acoustic parameters and spectroscopic methods. *Physics and Chemistry of Liquids, 52*, 331–341. http://dx.doi.org/10.1080/00319104.2013.830222