

Ultrasonic behavior of various chalcones in some solvents at different temperatures

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SUMMARY

Ultrasonic velocity, density and viscosity of some synthesized chalcones were measured in N,N-dimethyl formamide and chloroform at different temperatures (298.15 to 318.15 K). From these experimental data, various acoustical parameters such as specific impedance (Z), adiabatic compressibility (κ_s), Rao's molar sound function (R_m), intermolecular free path length (L_f), solvation number (S_n), internal pressure (π) have been calculated in order to understand the molecular interactions in the studied solutions. The results are interpreted in terms of molecular interactions occurring in the solutions.

Keywords: Ultrasonic velocity, chalcones, acoustical parameters, DMF, chloroform.

SUMMARY

Comportamiento ultrasónico de varias chalconas en algunos disolventes a diferentes temperaturas

La velocidad ultrasónica, la densidad y la viscosidad de soluciones de algunas chalconas sintéticas se midieron en N, N-dimetilformamida y cloroformo a diferentes temperaturas (desde 298,15 hasta 318,15 K). A partir de estos datos experimentales, se calcularon diversos parámetros acústicos tales como la impedancia específica (Z), la compresibilidad adiabática (κ_s), la función de sonido molar de Rao (R_m), la longitud de trayecto libre intermolecular (L_f), el número de solvatación (S_n) y la presión interna (π), para comprender las interacciones moleculares en las soluciones

estudiadas. Los resultados se interpretan en términos de las posibles interacciones moleculares que ocurren en las soluciones.

Palabras clave: Velocidad ultrasónica, chalconas, parámetros acústicos, DMF, cloroformo.

INTRODUCTION

Ultrasonic, a versatile non-destructive technique is a subject of extensive research because of its applications in various fields such as biology, medicine, in chemical industries, consumer industries, medical field, physics, etc. [1-9]. Further, now a days, ultrasonic waves are used in chemical and food processing industries [10-13].

The study of ultrasonic velocity along with density and viscosity at different temperatures and concentrations has been used to draw conclusion about molecular interactions, complex formation, etc. [14-16]. The ultrasonic technique is highly sensitive to molecular interactions and it gives valuable information about nature and strength of molecular interactions in solutions.

Chalcones are an important class of biologically active compounds which are known to exhibit a wide spectrum of biological and pharmacological activities like antispasmodic, anti-helminthics, anti-inflammatory, antiviral, ant allergic, antifungal, antibacterial, anticancer, anti-tubercular, anti-HIV, antioxidant, etc. [17-27].

Owing to vast biological and pharmacological applications of chalcones, it would be interesting to study acoustical properties of such compounds. The obtained data may be useful to scientists for Quantitative Structure Activity Relationship (QSAR) study of these compounds.

Thus, in the present work, some new chalcones are synthesized and their structure characterization was done by IR, ^1H NMR and mass spectral data. The density, ultrasonic velocity and viscosity of these synthesized compounds were measured in N,N-dimethyl formamide and chloroform over a wide range of concentration at different temperatures. From these experimental data, various acoustical parameters such as specific impedance (Z), adiabatic compressibility (χ_s), Rao's molar sound function (R_m), inter molecular free path length (L_f), solvation number (S_n), internal pressure (π) have been calculated. The obtained results are discussed in term of solute-solute and solute-solvent interactions occurring in the studied solutions.

EXPERIMENTAL

Materials

α -tetralone, methanol, 4-fluoro benzaldehyde and 4-methyl benzaldehyde used in the synthesis were supplied from Spectrochem Pvt. Ltd. (Mumbai, India). The solvents, DMF and chloroform used in the present work were of AR grade supplied by LOBA Chemie Pvt. Ltd. (Mumbai, India) and were purified according to the standard reported method [28]. The purified solvents were kept over molecular sieves. The final purities of the solvents were checked by GC-MS (SHIMADZU-Model No.-QP-2010).

Synthesis

Equimolar mixture of α -tetralone and substituted benzaldehydes in ethanol was refluxed for 4 h in presence of catalytic amount of potassium hydroxide. The reaction progress was checked by analytical thin layer chromatography (TLC) using (4:1-Hexane: Ethyl acetate) as mobile phase. After completion of reaction, the temperature of reaction mass was allowed cool up to room temperature and the resulting solid was filtered, washed with water and was dried under vacuum to give crude product. The obtained crude product was purified by washing with diethyl ether.

The reaction scheme is given in figure 1.

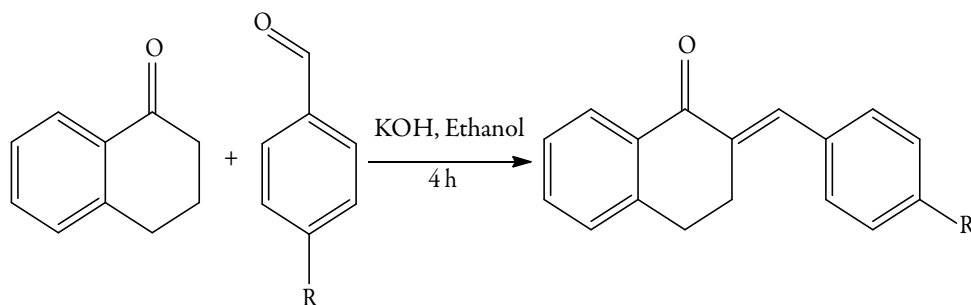


Figure 1. Reaction scheme for the synthesis of chalcones

Overall, two compounds were synthesized and the IUPAC names of these compounds are:

SB-1:2-(4-fluorobenzylidene)-3,4-dihydro naphthalene-1,(2*H*)-one.

SB-2:2-(4-methylbenzylidene)-3,4-dihydro naphthalene-1,(2*H*)-one.

Spectroscopy study

The structure of the synthesized compounds was confirmed by IR, ¹H NMR and mass spectral analysis. The IR spectra of compounds were taken on FT-IR (SHIMADZU Model-IRaffinity-1S). ¹H NMR spectra were taken on a Bruker AVANCE III (400 MHz). In all the cases, ¹H NMR spectra were obtained in deuterated dimethyl sulfide (DMSO-d₆) using TMS as an internal standard. The NMR signals are reported in δ ppm. Mass spectra were determined using direct inlet probe on a GC-MS (SHIMADZU Model-QP2010) mass spectrometer.

The melting points of compounds were measured by Different Scanning Calorimeter (SHIMADZU DSC-60) under nitrogen atmosphere.

Measurements of density, ultrasound velocity and viscosity

Measurements of density and ultrasound velocity

The solutions of chalcones were prepared in DMF and chloroform in the concentration range from 0.01 to 0.10 mol.L⁻¹ and were stored in bottles with PTFE septum until further use. The standard uncertainties of solutions are 0.0001 mol.L⁻¹. An electronic balance (Mettler Toledo Model-AB204-S) with accuracy of ±0.0001 g was used for weighing.

The density and ultrasonic velocity of pure solvents and solutions were measured at different temperatures (298.15, 308.15 and 318.15 K) using Anton Paar Density and Sound velocity meter (DSA 5000M). The temperature was controlled up to ± 0.01 K by a built-in Peltier device. Before measurements, the instrument DSA 5000M was calibrated by ultra-pure water in the experimental temperature range. The standard uncertainty of the density and ultrasonic velocity was found to be 0.5 kg.m⁻³ and 0.5 m.s⁻¹, respectively.

Measurement of viscosity

To determine the viscosity of pure solvents and solutions, Ubbelohde viscometer was used. The measured quantity of the distilled water / solvent / solution was placed in the viscometer, which was suspended in a constant temperature bath (NOVA Instruments Pvt. Ltd.-Ahmedabad) (NV-8550 E) at definite temperature. The accuracy of bath was $\pm 0.5^\circ \text{C}$. A digital stop watch (Hanhart-Germany) with accuracy of ± 0.01 second was used to determine flow time of solutions. Using the flow times (t) and known viscosity of standard water sample, the viscosity of solvent and solutions were determined according to equation:

$$\frac{\eta_1}{\eta_2} = \frac{t_1 \rho_1}{t_2 \rho_2} \quad (1)$$

where η_1 and η_2 are the viscosities of water and solutions respectively; t_1 and ρ_1 are the flow of time and density of water whereas t_2 and ρ_2 are the flow of time and density of solutions respectively.

RESULTS AND DISCUSSION

Table 1 shows the substitutions and other physical properties of synthesized compounds.

Table 1. Physical constants of the synthesized compounds.

Compound	Mol. Formula	Mol. Wt. (g.mol ⁻¹)	% Yield	R _f *value	Melting point (K)
SB-1	C ₁₇ H ₁₃ FO	252.12	78	0.49	386.15
SB-2	C ₁₈ H ₁₆ O	248.31	74	0.36	395.81

*4:1-Hexane: Ethyl acetate

Spectral Data:

Figures 2 and 3 show IR and ¹H NMR of synthesized compounds.

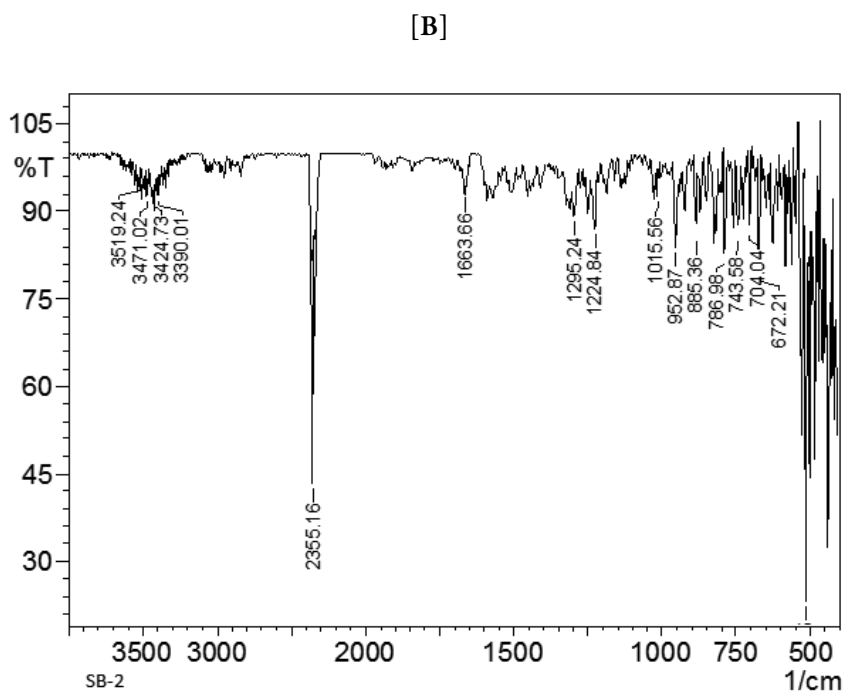
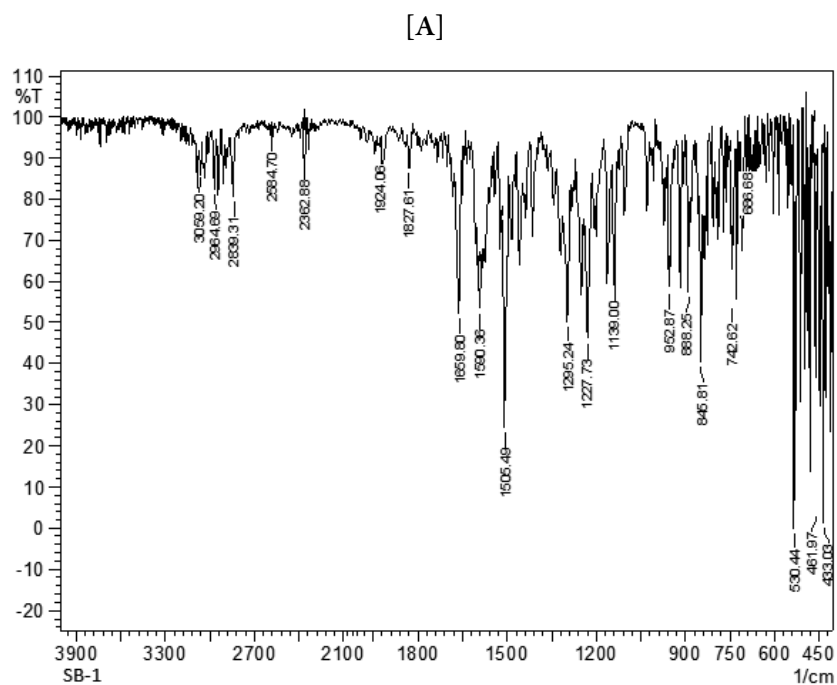
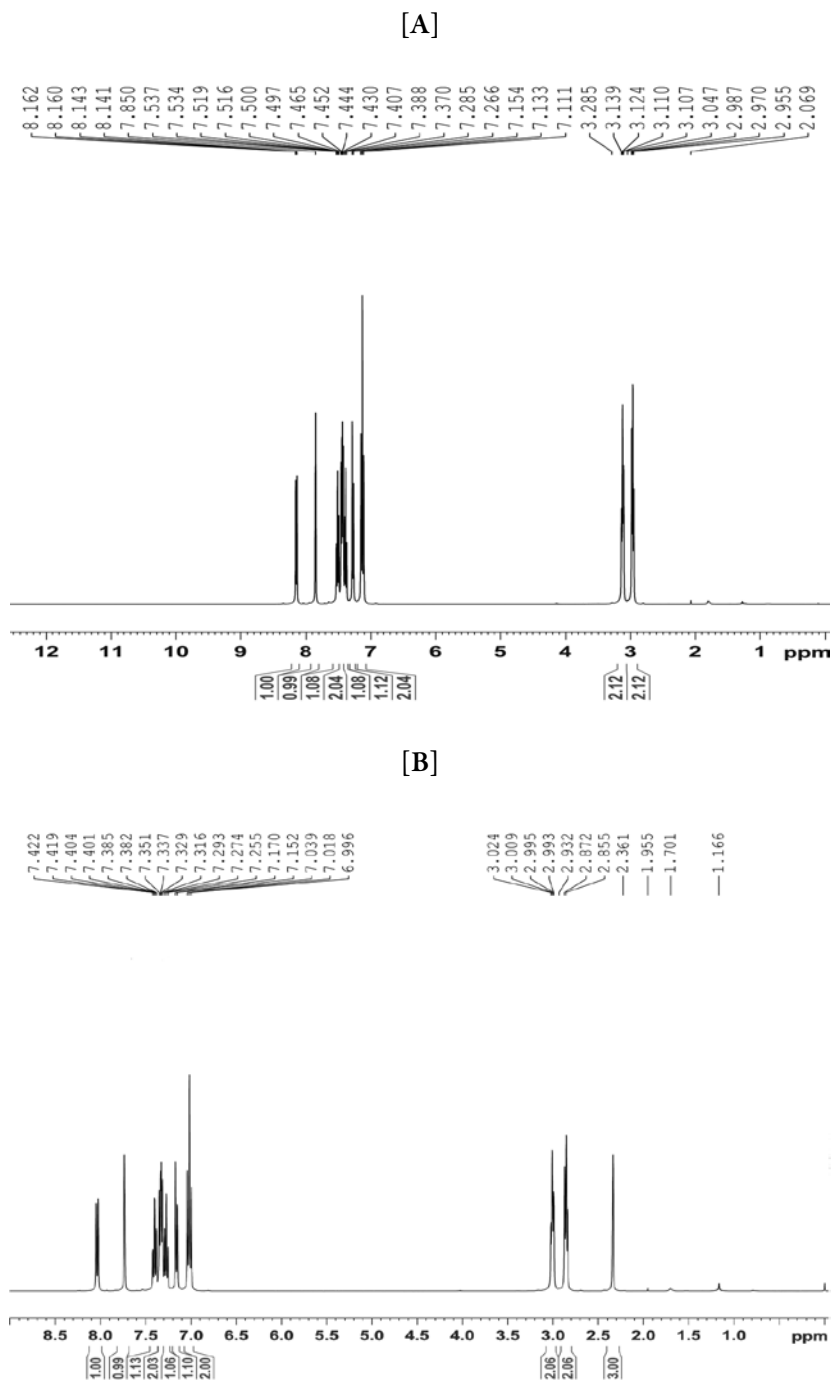


Figure 2: IR spectra of [A] SB-1 and [B] SB-2


 Figure 3: ^1H -NMR spectra of [A] SB-1 and [B] SB-2

SB-1:

IR (cm^{-1} , *KBr*): 3059.20 (Ar-H asym. stretching), 2964.69-2839.31 (CH_2 stretching of cyclohexanone ring), 1659.80 (C = O stretching), 1295.24-1227.73 ($-CH_2$ bending), 952.87 (ring stretching in cyclohexanone), 845 (C-H out of plane bending), 1139 (C-F stretching).

1H NMR ($CDCl_3$) $\delta(ppm)$: 2.955-2.987 (2H, triplet, $J = 6.4$), 3.107-3.139 (2H, triplet, $J = 6.4$), 7.111-7.154 (2H, triplet, $J = 8.6$), 7.266-7.285 (1H, doublet, $J = 7.6$), 7.370-7.389 (1H, triplet, $J = 3.8$), 7.408-7.466, (2H, quartet), 7.497-7.537 (1H, triplet, $J = 8.0$), 7.851 (1H, Singlet), 8.141-8.162 (1H, doublet, $J = 8.4$).

MS: (m/z) = 252.12

SB-2:

IR (cm^{-1} , *KBr*): 3050.52 (Ar-H asym. str.), 2846.06 (CH_2 stretching of cyclohexanone ring), 1663.80 (C = O stretching), 1295.24-1224.73 ($-CH_2$ bending), 952.87 (ring stretching in cyclohexanone), 845 (C-H out of plane bending), 2951.19 ($-CH_3$ stretching).

1H NMR ($CDCl_3$) $\delta(ppm)$: 2.361 (3H, singlet) 2.855-2.932 (2H, triplet, $J = 6.4$), 2.993-3.024 (2H, triplet, $J = 6.4$), 6.996-7.152 (2H, triplet, $J = 8.6$), 7.170-7.255 (1H, doublet, $J = 7.6$), 7.274-7.316 (1H, triplet, $J = 3.8$), 7.329-7.351 (2H, quartet), 7.382-7.385 (1H, triplet, $J = 8.0$), 7.401-7.404 (1H, Singlet), 7.419-7.422 (1H, doublet, $J = 8.4$).

MS: (m/z) = 248.32

Table 2. Experimental data of density, ultrasonic velocity and viscosity of chalcones in chloroform and N,N-dimethyl formamide at different temperatures.

Conc. M	Density (Kg.m ⁻³)	Velocity (m.s ⁻¹)	Viscosity (mPa.s)	Density (Kg.m ⁻³)	Velocity (m.s ⁻¹)	Viscosity (mPa.s)
SB-1						
Chloroform				DMF		
298.15 K						
0.00	1479.32	983.90	0.7678	943.94	1457.71	0.8158
0.01	1478.65	985.01	0.7529	945.58	1461.57	0.8608
0.02	1478.11	986.11	0.7559	946.43	1462.97	0.8571
0.04	1476.99	987.98	0.7581	947.65	1463.64	0.8552
0.06	1476.04	989.58	0.7647	948.70	1464.44	0.8549
0.08	1475.26	991.15	0.7699	949.54	1465.03	0.8511
0.10	1474.55	992.67	0.7761	949.77	1466.34	0.8396
308.15 K						
0.00	1460.15	949.94	0.6837	934.38	1418.80	0.7011
0.01	1459.54	951.07	0.6843	936.02	1422.74	0.7498
0.02	1459.03	952.12	0.6897	936.88	1424.11	0.7472
0.04	1458.01	953.98	0.6936	938.98	1425.83	0.7418
0.06	1457.30	955.69	0.6959	939.16	1426.64	0.7391
0.08	1456.40	957.11	0.6968	940.00	1427.26	0.7319
0.10	1455.76	958.75	0.7004	940.23	1428.58	0.7295
318.15 K						
0.00	1440.27	916.11	0.6129	924.77	1380.15	0.6337
0.01	1440.18	917.25	0.6152	926.42	1384.19	0.6745
0.02	1439.71	918.30	0.6203	927.28	1385.60	0.6722
0.04	1438.77	920.23	0.6252	928.50	1386.29	0.6640
0.06	1438.11	921.23	0.6273	929.57	1387.79	0.6613
0.08	1437.31	923.39	0.6282	930.42	1388.56	0.6559
0.10	1436.74	925.06	0.6332	930.64	1389.31	0.6490

(keep going)

Table 2. Experimental data of density, ultrasonic velocity and viscosity of chalcones in chloroform and N,N-dimethyl formamide at different temperatures (*continuation*)

Conc. M	Density (Kg.m ⁻³)	Velocity (m.s ⁻¹)	Viscosity (mPa.s)	Density (Kg.m ⁻³)	Velocity (m.s ⁻¹)	Viscosity (mPa.s)
SB-2						
Chloroform				DMF		
298.15 K						
0.00	1478.99	983.92	0.7676	943.94	1457.71	0.8158
0.01	1477.99	984.77	0.7554	946.12	1465.31	0.7717
0.02	1477.26	985.71	0.7597	946.95	1467.22	0.7697
0.04	1475.91	987.32	0.7632	947.77	1468.01	0.7677
0.06	1474.72	988.84	0.7668	948.21	1468.97	0.7635
0.08	1473.63	990.20	0.7733	948.83	1469.36	0.7601
0.10	1472.85	991.35	0.7836	949.41	1470.19	0.7551
308.15 K						
0.00	1459.83	949.94	0.6835	934.38	1418.80	0.7011
0.01	1458.89	950.89	0.6757	936.57	1426.54	0.7396
0.02	1458.20	951.80	0.6797	937.41	1428.48	0.7681
0.04	1456.12	953.45	0.6818	938.25	1429.23	0.7657
0.06	1455.80	954.98	0.6871	938.70	1430.17	0.7599
0.08	1454.78	956.33	0.6924	939.17	1431.55	0.7574
0.10	1454.05	957.49	0.7019	939.82	1432.32	0.7540
318.15 K						
0.00	1440.27	916.11	0.6129	924.77	1380.15	0.6337
0.01	1439.52	917.05	0.6117	926.98	1388.02	0.6699
0.02	1438.88	918.00	0.6151	927.82	1389.96	0.6682
0.04	1437.69	919.67	0.6207	928.67	1390.72	0.6664
0.06	1436.64	921.25	0.6255	929.14	1391.69	0.6629
0.08	1435.68	922.57	0.6287	929.41	1392.05	0.6596
0.10	1435.00	923.78	0.6312	930.27	1393.12	0.6555

Table 2 shows experimental density, ultrasonic velocity and viscosities of pure solvents and solutions of both the compounds. From the experimental data of density, viscosity and ultrasonic velocity, various acoustical parameters such as specific acoustical

impedance (Z), adiabatic compressibility (κ_s), intermolecular free path length (L_f), Rao's molar sound function (R_m), free volume (V_f), internal pressure (π), solvation number (S_n) etc. are evaluated using following equations:

Specific acoustical impedance (Z):

$$Z = Up \quad (2)$$

Adiabatic compressibility (κ_s):

$$\kappa_s = \frac{1}{U^2 \rho} \quad (3)$$

Intermolecular free path length (L_f) [29]:

$$L_f = \kappa_j \kappa_s^{1/2} \quad (4)$$

where K_j is Jacobson constant ($=2.0965 \times 10^{-6}$)

Rao's molar sound function (R_m) [30]:

$$R_m = \left(\frac{M}{\rho} \right) U^{1/3} \quad (5)$$

where M is the apparent molecular weight of solution and can be calculated according to the following equation:

$$M = M_1 W_1 + M_2 W_2 \quad (6)$$

where W_1 and W_2 are weight fractions of solvent and solute respectively. M_1 and M_2 are molecular weights of the solvent and solute respectively.

Free volume (V_f) [31]:

$$V_f = \left[\frac{M U}{K \eta} \right]^{3/2} \quad (7)$$

Internal pressure (π) [32]:

$$\pi = b R T \left[\frac{K_n}{U} \right]^{1/2} \frac{\rho^{2/3}}{M^{1/6}} \quad (8)$$

Solvation number (S_n) [31]:

$$S_n = \frac{M_2}{M_1 \left[1 - \frac{Ka}{Ka1} \right] \left[\frac{(100 - X)}{X} \right]} \quad (9)$$

where X is the number of grams of solute in 100 g of the solution. M_1 and M_2 are the molecular weights and κ_{a1} and κ_a are adiabatic compressibility of solvent and solute respectively.

Some of these evaluated parameters are reported in table 3.

Table 3. Some acoustical parameters of SB-1 in chloroform and N,N-dimethyl formamide at different temperatures.

Conc. M	$Z, 10^{-6}$ Kg.m ⁻² .s ⁻¹	$V_f, 10^{12}$ m ³	$R_m, 10^4$ m ^{-8/3} .s ^{1/3}	$\pi, 10^{-10}$ Pa	$Z, 10^{-6}$ Kg.m ⁻² .s ⁻¹	$V_f, 10^{12}$ m ³	$R_m, 10^4$ m ^{-8/3} .s ^{1/3}	$\pi, 10^{-10}$ Pa
Studied compounds								
Chloroform					DMF			
298.15K								
0.00	1.4555	3.0586	8.0264	1.4042	1.3760	2.8942	8.7795	1.5623
0.01	1.4565	2.9835	8.0483	1.3862	1.3820	3.1801	8.8294	1.5923
0.02	1.4576	3.0149	8.0695	1.3848	1.3846	3.1948	8.8814	1.5772
0.04	1.4592	3.0543	8.1112	1.3788	1.3870	3.2480	8.9853	1.5531
0.06	1.4607	3.1190	8.1515	1.3769	1.3893	3.3110	9.0906	1.5309
0.08	1.4622	3.1763	8.1909	1.3740	1.3911	3.3530	9.1972	1.5062
0.10	1.4637	3.2402	8.2297	1.3720	1.3927	3.3504	9.3113	1.4742
308.15K								
0.00	1.3871	2.4382	8.0371	1.3817	1.3257	2.2141	8.790	1.507
0.01	1.3881	2.4527	8.0591	1.3780	1.3317	2.4834	8.840	1.546
0.02	1.3892	2.4934	8.0804	1.3793	1.3342	2.4980	8.893	1.532
0.04	1.3909	2.5364	8.1223	1.3751	1.3388	2.5238	8.992	1.505
0.06	1.3927	2.5705	8.1622	1.3695	1.3398	2.5607	9.107	1.480
0.08	1.3939	2.5959	8.2024	1.3628	1.3416	2.5728	9.215	1.452
0.10	1.3957	2.6379	8.2419	1.3587	1.3432	2.6120	9.330	1.428

(keep going)

Table 3. Some acoustical parameters of SB-1 in chloroform and N,N-dimethyl formamide at different temperatures (*continuation*).

Conc. M	$Z, 10^{-6}$ Kg.m ⁻² .s ⁻¹	$V_f 10^{12}$ m ³	$R_m, 10^4$ m ^{8/3} .s ^{1/3}	$\tau, 10^{-10}$ Pa	$Z, 10^{-6}$ Kg.m ⁻² .s ⁻¹	$V_f 10^{12}$ m ³	$R_m, 10^4$ m ^{8/3} .s ^{1/3}	$\tau, 10^{-10}$ Pa
Studied compounds								
Chloroform				DMF				
318.15K								
0.00	1.3194	1.9597	8.0501	1.3628	1.2763	1.8254	8.7996	1.4895
0.01	1.3210	1.9806	8.0697	1.3615	1.2823	2.0332	8.8512	1.5243
0.02	1.3221	2.0144	8.0911	1.3629	1.2848	2.0463	8.9045	1.5103
0.04	1.3240	2.0565	8.1335	1.3600	1.2872	2.0499	9.0108	1.4793
0.06	1.3248	2.0825	8.1717	1.3551	1.2900	2.0806	9.1199	1.4548
0.08	1.3272	2.1063	8.2143	1.3479	1.2919	2.0962	9.2294	1.4280
0.10	1.3291	2.1497	8.2541	1.3456	1.2929	2.1040	9.3450	1.3997
SB-2								
298.15 K								
0.00	1.4552	3.0577	8.0282	1.4038	1.3760	2.8942	8.7795	1.5623
0.01	1.4555	2.9968	8.0506	1.3884	1.3864	2.7090	8.8297	1.5068
0.02	1.4561	3.0351	8.0717	1.3883	1.3894	2.7289	8.8809	1.4938
0.04	1.4572	3.0804	8.1128	1.3837	1.3913	2.7710	8.9848	1.4710
0.06	1.4583	3.1263	8.1529	1.3793	1.3929	2.8019	9.0924	1.4463
0.08	1.4592	3.1895	8.1921	1.3777	1.3942	2.8347	9.1970	1.4235
0.10	1.4601	3.2770	8.2291	1.3798	1.3958	2.8597	9.3026	1.3995

(keep going)

Table 3. Some acoustical parameters of SB-1 in chloroform and N,N-dimethyl formamide at different temperatures (continuation).

Conc. M	$Z \cdot 10^{-6}$ Kg.m ⁻² .s ⁻¹	$V_f \cdot 10^{12}$ m ³	$R_m \cdot 10^4$ m ^{-8/3} .s ^{1/3}	$\pi \cdot 10^{-10}$ Pa	$Z \cdot 10^{-6}$ Kg.m ⁻² .s ⁻¹	$V_f \cdot 10^{12}$ m ³	$R_m \cdot 10^4$ m ^{-8/3} .s ^{1/3}	$\pi \cdot 10^{-10}$ Pa
Studied compounds								
Chloroform					DMF			
308.15 K								
0.00	1.3868	2.4374	8.0389	1.3814	1.3257	2.2141	8.7897	1.5070
0.01	1.3872	2.4055	8.0615	1.3692	1.3361	2.4416	8.8409	1.5346
0.02	1.3879	2.4374	8.0827	1.3692	1.3391	2.6140	8.8927	1.5524
0.04	1.3883	2.4686	8.1287	1.3630	1.3410	2.6528	8.9976	1.5281
0.06	1.3903	2.5169	8.1628	1.3613	1.3425	2.6739	9.1063	1.5006
0.08	1.3912	2.5658	8.1848	1.3612	1.3445	2.7138	9.2157	1.4769
0.10	1.3922	2.6380	8.2141	1.3643	1.3461	2.7464	9.3218	1.4535
318.15 K								
0.00	1.3194	1.9597	8.0501	1.3628	1.2763	1.8254	8.7996	1.4895
0.01	1.3201	1.9628	8.0721	1.3575	1.2867	2.0203	8.8518	1.5181
0.02	1.3209	1.9876	8.0935	1.3571	1.2896	2.0360	8.9043	1.5048
0.04	1.3222	2.0314	8.1353	1.3554	1.2915	2.0683	9.0103	1.4815
0.06	1.3235	2.0718	8.1761	1.3529	1.2931	2.0923	9.1203	1.4563
0.08	1.3245	2.1039	8.2158	1.3490	1.2938	2.1165	9.2307	1.4322
0.10	1.3256	2.1326	8.2536	1.3446	1.2960	2.1376	9.3364	1.4081

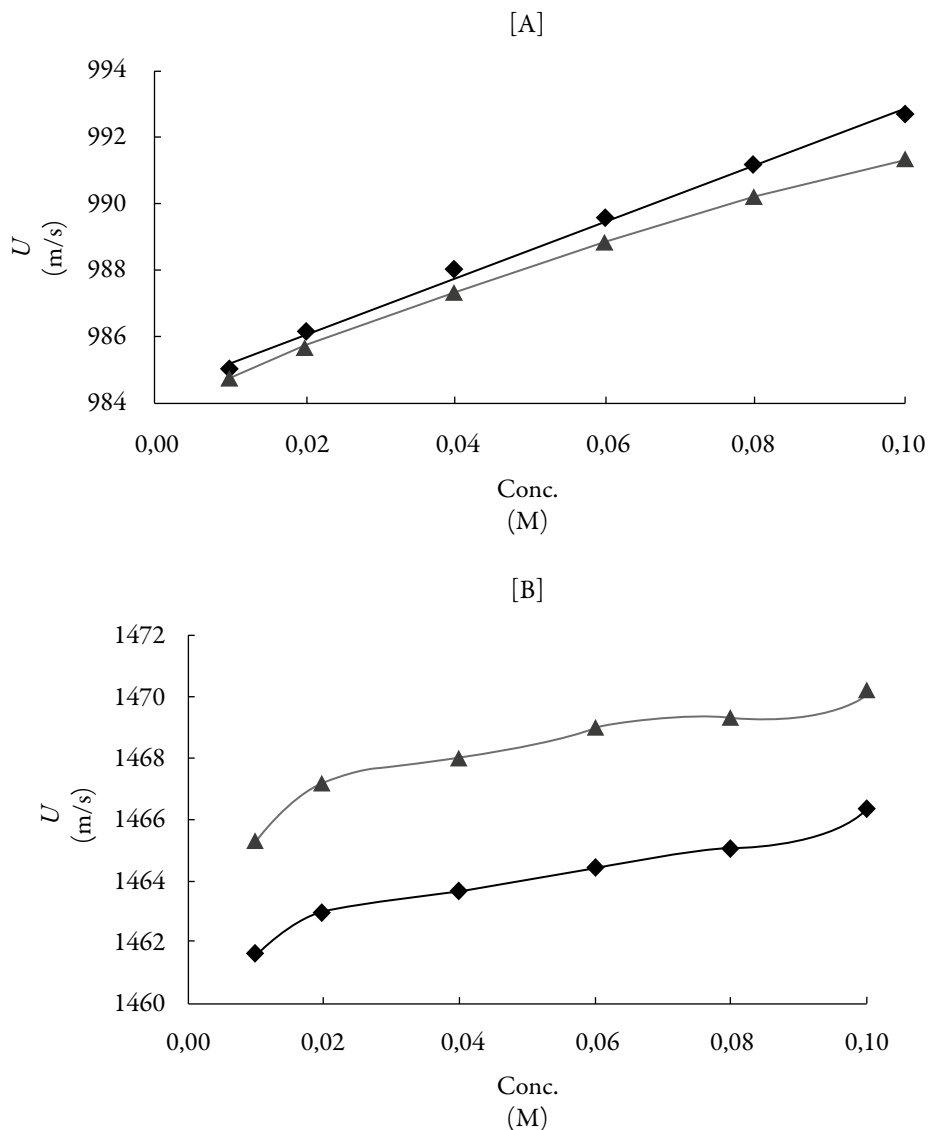


Figure 4. The variation of ultrasonic velocity (U) with concentration for the studied compounds in [A] chloroform and [B] DMF at 298.15 K. SB-1, (\blacklozenge); SB-2, (\blacktriangle).

Figure 4 shows the variation of ultrasonic velocity with concentration for the studied compounds in both the solvents. It is observed from Figure 4 that the velocity increases almost linearly with concentration for both SB-1 and SB-2 in chloroform whereas in dimethyl formamide, the increase is non-linear. Further, the velocity is higher in DMF

than that in chloroform. The increase of velocity is related to intermolecular free path length (L_f) which is found to decrease with concentration in both the solvents as shown in Figure 5. Again, the decrease is linear in chloroform and non-linear in dimethyl formamide for both the compounds. Thus, velocity is reciprocal of intermolecular free path length. The decrease of L_f suggests that compound and solvent molecules interact with each other i.e., compound-solvent interactions takes place in solution. This causes decrease in distance between compound and solvent molecules causing thereby an increase in velocity.

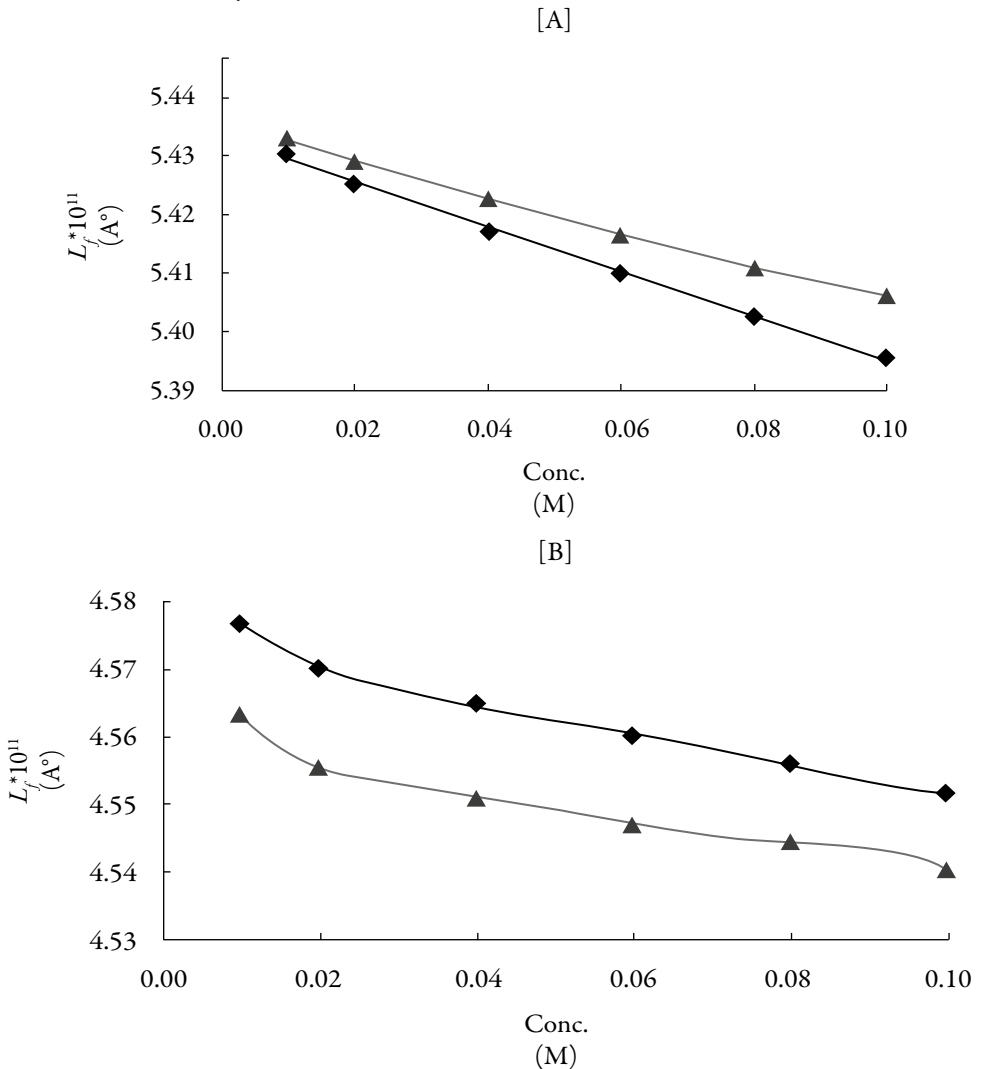


Figure 5. The variation of free path length (L_f) with concentration of the studied compounds in [A] chloroform and [B] DMF at 298.15 K. SB-1, (\blacklozenge); SB-2, (\blacktriangle).

Figure 6 shows that the variation of adiabatic compressibility (κ_s) with concentration which is again found to decrease with concentration for both compounds in both the solvents. This further confirms the existence of compound-solvent interactions in studied systems. The predominance of solute-solvent interaction is further proved by increase of specific impedance (Z) (table 3).

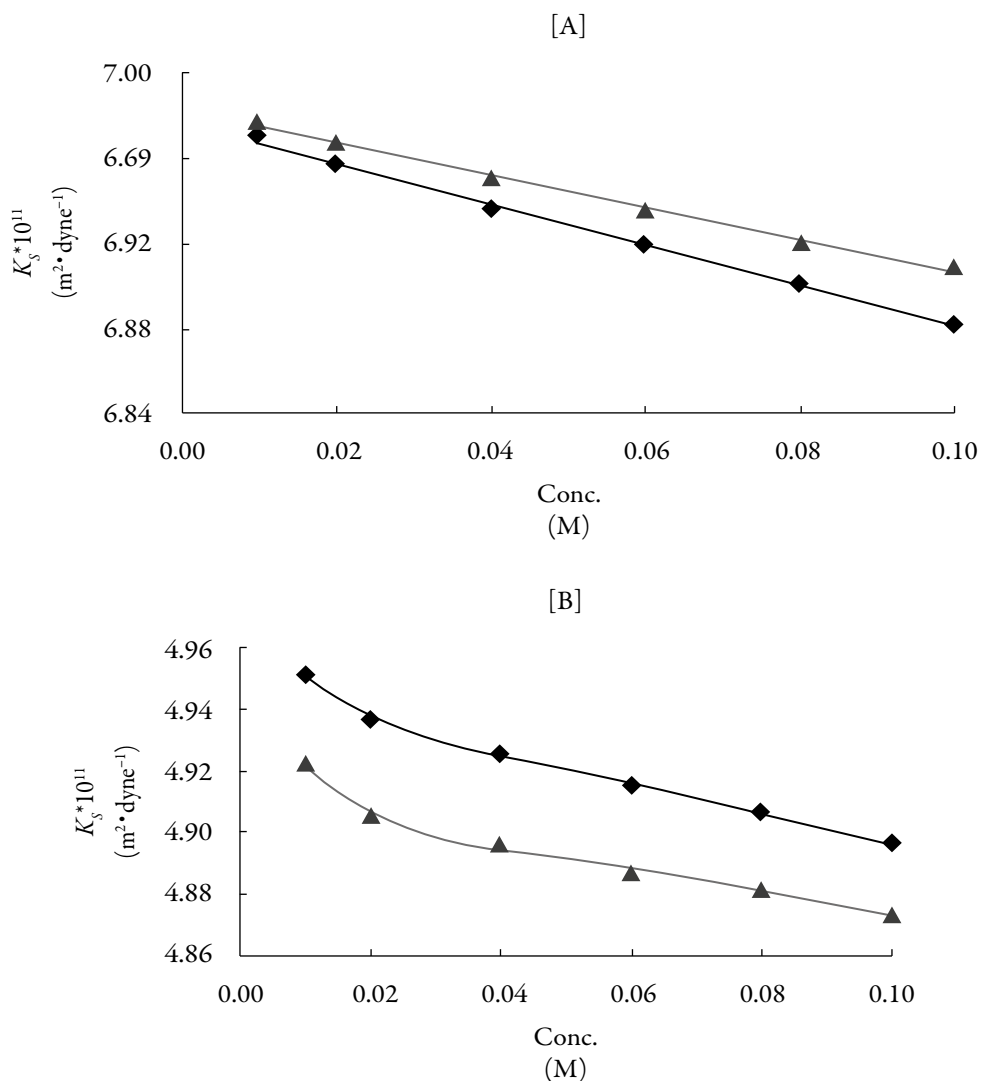
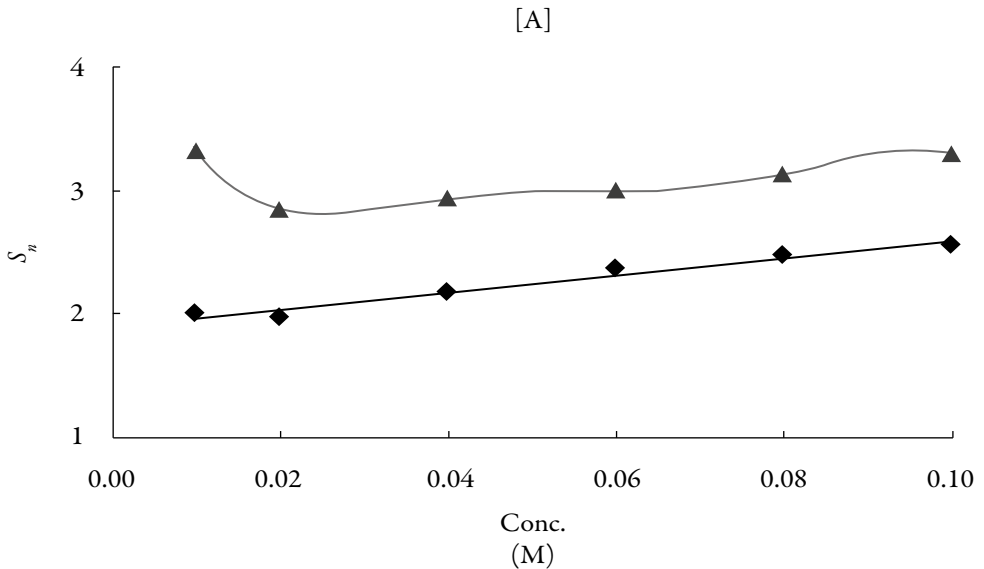


Figure 6. The variation of adiabatic compressibility (κ_s) with concentration for studied compound in [A] Chloroform and [B] DMF at 298.15 K. SB-1, (\blacklozenge); SB-2, (\blacktriangle).

Table 3 shows that Rao's molar function increases continuously for all the solutions for both the compounds indicating thereby that there is no complex formation in the studied solutions. The internal pressure (π) is a measure of cohesive energy in the solution which is found to decrease. This suggests that in the studied systems, compound-compound interactions also exist. This is again suggested by increase in free volume which is found to increase. However, the decrease of internal pressure and increase in free volume is in very small magnitude. Thus, in the studied systems, both compound-solvent and compound-compound interactions are present but their magnitudes are much different.

The magnitude and type of interactions are also predicted by a parameter Solvation number which is a measure of structure forming or structure breaking tendency of solute in a particular solvent. Figure 7 shows the variation of solvation number (S_n) with concentration. It is observed from figure 7 that solvation number increases with concentration for both the compounds and are found to be positive. The positive values of solvation number suggest structure forming tendency of the studied compounds in the studied solvents. This again proves that in studied solutions, compound-solvent interactions dominate.



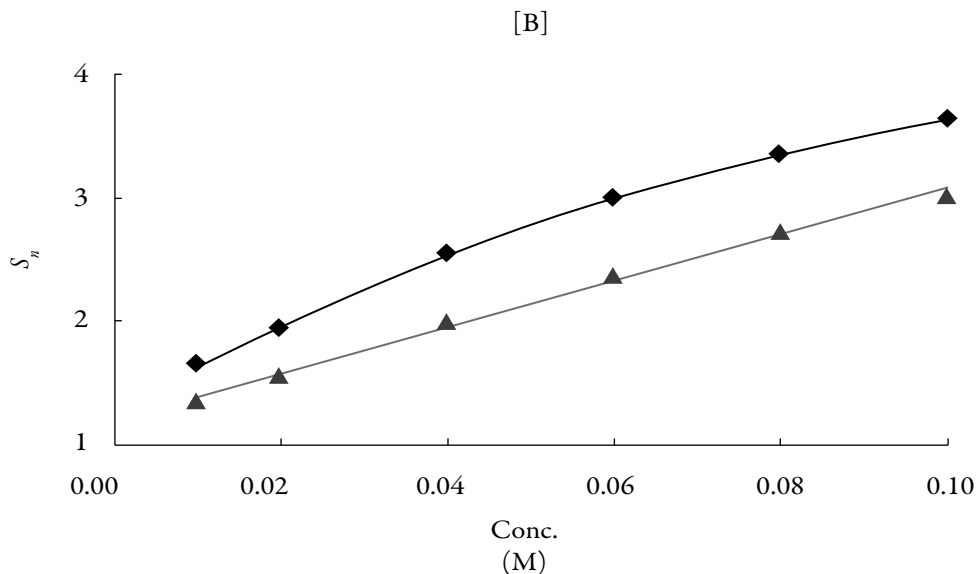


Figure 7. The variation of solvation number (S_n) with concentration for the studied compounds in [A] Chloroform and [B] DMF at 298.15 K. SB-1, (\blacklozenge); SB-2, (\blacktriangle).

CONCLUSION

On the bases of the evaluated data, it is concluded that in both chloroform and DMF, predominance of compound-solvent interactions exist for both the compounds. Further, interactions increases with increase in concentration but decreases with increase in temperature. In DMF, high values of ultrasonic velocity are observed. “However, in chloroform reverse order of compounds for ultrasonic velocity is obtained, indicating thereby that compound SB-2 containing 4-methyl group causes strong solute-solvent interactions in chloroform than 4-fluoro group (as in SB-1).

DISCLOSURE STATEMENT

No potential conflict of interest was reported by the authors.

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