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Ultrasonic Studies and Molecular Interactions of N, N-Dimethyl Formamide and 1-Butanol with n-Hexane at Different Temperatures 303K ,308K and 313K.

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ABSTRACT

The Ultrasonic velocity(U), density(ρ), and viscosity(η) have been measured for the ternary liquid mixtures of N,N-Dimethyl Formamide (NNDMF), 1 butanol and n hexane at various temperatures viz., 303 k,308 k and 313 k at constant frequency 2 MHz. for different concentrations ranges from 0.001M to 0.01M. The acoustical parameters such as adiabatic compressibility(β), Rao constant(R), absorption coefficient (α/f^2), internal pressure(π_i), cohesive energy(CE), free volume(V_f), free length(L_f) and acoustic impedence(z), were calculated from the experimental data. These para
meters in accordance with their ultrasonic velocities corresponding to different concentrations were discussed.

Keywords: molecular interactions, ultrasonic velocity, ternary liquid mixture, adiabatic compressibility, internal pressure, acoustic impedence.

1. INTRODUCTION

Ultrasonic investigation of liquid mixture containing polar-polar and nonpolar components is of considerable significances in understanding intermolecular interaction between the component molecules as that finds application in several industrial and technological processes [1]. Ultrasonic velocity and the derived acoustical parameters like adiabatic compressibility, free length, relaxation time, acoustic impedance, etc., provide valuable information about the molecular interactions. This has been studied for various binary and ternary liquid mixtures [2-7] with respect to variation in concentration of the liquid mixtures and temperatures. In the present paper, variation of different parameters of ternary liquid mixtures containing N,N-dimethylformamide (N,N-DMF), 1 butanol and n hexane with respect to different temperatures such as 303K, 308K and 313K have been studied for different concentrations.

N,N-Dimethl formamide is a non-aqueous solvent which has no hydrogen bonding in pure state. Therefore it acts as an aprotic, protophilic medium with high dielectric constant. N,N DMF

is a polar molecule having a dipole moment, when it is associated with 1 butanol, the dipole-dipole interaction dominates the dipole-induced dipole interaction. The relatively small size of N,N-DMF and its linear aliphatic configuration may be the factor contributing to the volume contraction of the mixture. N,N DMF is used as solvent in various fields like medicinal, chemical industries, pharma industries etc., this property prompted the author to undertake the present study. 1 Butanol is relatively a linear molecule, and its non-ideality in all probabilities may be due to the polarity arising out of C-N and O-H bonds. As far as the O-H group is concerned, it rotates freely along the C-N axis which is likely to give more flexibility to the interaction arises due to polar O-H and N-O bonds. n Hexane belongs to the aliphatic hydrocarbon. It is highly inert towards an electrophile or nucleophile at ordinary temperature. n Hexane being non polar is not expected to be involved in any strong interaction with the other components of the mixture [8]. However, dispersive types of interactions are possible between them.

2. EXPERIMENTAL SETUP

The mixtures of various equimolar concentrations were prepared by taking analytical reagent grade and spectroscopic reagent grade chemicals with minimum assay of 99.9% and obtained from E.Merck Ltd (India). All the component liquids were purified by the standard methods [9-12]. The density, viscosity, and ultrasonic velocity were measured as a function of concentration of the ternary liquid mixture at 303k, 308k and 313k. Ultrasonic velocity measurements were made using an ultrasonic interferometer (Model F-81, supplied by M/S Mittal Enterprises, New Delhi) with the accuracy of ±0.1m·s−1. An electronically operated digital constant temperature bath (Model SSI-03 Spl, supplied by M/S Mittal Enterprises, New Delhi), operating in the temperature range of −10°C to 85°C with an accuracy of ±0.1°C has been used to circulate water through the outer jacket of the double-walled measuring cell containing the experimental liquid. The densities of the mixture were measured using a 10-ml specific gravity bottle by relative measurement method with an accuracy of ±0.01 kg·m−3. An Oswald viscometer (10 ml) with an accuracy of ±0.001 Ns·m−2 was used for the viscosity measurement. The flow time was determined using a digital racer stopwatch with an accuracy of ±0.1s.

2.1 Theory and Calculations

Intermolecular free length (L_f), is calculated using the standard expression

$$L_f = KT\ \beta^{1/2} \qquad (1)$$

Where KT is a temperature dependent constant known as Jacobson constant {K = (93.875 + 0.375 T) × 10^{-8} } and β is the adiabatic compressibility that can be calculated from the speed of sound (U) and the density of the medium (ρ) as

$$\beta = (u^2\rho)^{-1} \qquad (2)$$

The relation for free volume in terms of ultrasonic velocity and the viscosity (η) of liquid as

$$V_f = (M_{eff}\ U/\ k\eta)^{1/2} \qquad (3)$$

Expression for the determination of internal pressure π_i by the use of free volume as

$$\pi_i = bRT(K\eta/U)½(\rho^{2/3}/M^{7/6}_{eff}) \qquad (4)$$

Where b stands for cubic packing which is assumed to be 2 for liquids and K is a dimensionless constant independent of temperature and nature of liquids and its value is 4.281×10^9, T is the absolute temperature and M_{eff} is the effective molecular weight of the mixture. The viscous relaxation time was obtained by using the relation

$$\tau = (4/3)\, \beta\, \eta \qquad (5)$$

Gibbs free energy is calculated from the relation

$$\Delta G = KT \ln (KT\tau/h) \qquad (6)$$

Where τ is the viscous relaxation time, K the Boltzman constant, T, the absolute temperature and h is the Plancks constant.
The acoustic impendence is given by,

$$Z = U\rho \qquad (7)$$

Where U and ρ are the velocity and density of liquids respectively.

3. RESULTS AND DISCUSSION

The experimentally measured values of density, viscosity and ultrasonic velocity for the mixtures at 303, 308 and 313 K are presented in Table-1. Table-2,3 and 4 represents the free volume, cohesive energy and Gibbs free energy respectively. The values of adiabatic compressibility, intermolecular free length and internal pressure for the mixtures are depicted respectively in Table-3,4 and 5. Table-6,7 and 8 shows the computed values for acoustic impedance, relaxation time and absorption coefficient respectively for the mixtures at the three temperatures. From the Table-1, it was observed that the ultrasonic velocity of the ternary liquid mixtures decreases with increasing temperature at every concentration while it increases slowly at particular temperature when the concentration increases which is due to thermal agitation and compactness of the molecules respectively [13-14]. The density is found to increase with increasing the concentration and decreases with increase in temperature. However the viscosity increases with increases in temperature as well as in concentration.

The free volume is the average volume available in the system due to repulsion between the molecules. It was observed from the table 2 that free volume decreases like velocity with increase in temperature for every concentration which shows that the presence of molecular interaction. The same trend was also observed with respect to cohesive energy (table 3) which also supports the presence of molecular interaction. The Gibbs free energy (table 4) is found to be increases while the concentration increases at particular temperature which indicates that least interactions are possible between the donor-acceptor (ie NNDMF-1 Butanol). Similar observations are also received by Ali et al [15]. But when the temperature increases this value increases sharply at irrespective of concentrations and the –ve values also predict the less interactions.

Table 5 suggests that the free length decreases when the velocity increases while the concentration increases which gives idea regarding the less interactions. However the free length increases with increase in temperature which is due to dipole and induced dipole interactions. Adiabatic compressibility (table 6) decreases with increasing concentration of the liquid mixture which is in confirmation of the above fact. Internal pressure (table 7) is the measure of the totality of the forces and it contributes the cohesion/adhesion of the liquid system and from the values of internal pressure calculated, shows the force of cohesion increases.

Table 10, shows the acoustic impedence values along with the ultrasonic velocity values for the system provides valuable information about the dipole-dipole and dipole-induced dipole interactions between the NNDMF-1 butanol and the NNDMF-1butanol–n hexane interactions. These values support the weak interactions between the unlike molecules. The intermolecular free length as well as the relaxation time (table 8) play vital role in sound wave. These values increase with increase in temperature resulting weak interactions among molecules. The same inference has also been observed by Manoj kumar et al [15]. Table 9 shows the trend of absorption coefficient with respect to different temperatures.

Table 1. Experimental values of Velocity, Viscosity and Density

Sl. No.	Conc. (M)	Velocity (U) ms^{-1} at			Viscosity (η)$Nsm^{-2}X10^{-7}$at			Density (ρ) Kgm^{-3} at		
		303 K	308 K	313 K	303 K	308 K	313 K	303 K	308 K	313 K
1	0.001	1043.36	1026.52	1015.68	4.417	4.85	5.209	803	795	794
2	0.002	1043.82	1026.88	1015.78	4.416	4.86	5.234	801	795	794
3	0.003	1044.16	1027.16	1016.17	4.424	4.87	5.259	801	795	794
4	0.004	1045.12	1027.73	1016.93	4.432	4.87	5.293	801	793	794
5	0.005	1045.44	1028.12	1017.28	4.551	4.91	5.331	801	793	793
6	0.006	1046.06	1028.20	1017.62	4.566	4.93	5.338	803	795	793
7	0.007	1046.72	1028.70	1018.26	4.576	4.96	5.365	802	795	793
8	0.008	1047.11	1029.22	1018.72	4.597	4.98	5.397	803	796	793
9	0.009	1047.82	1030.72	101956	4.617	5.01	5.437	801	796	793
10	0.010	1048.24	1031.36	1019.92	4.681	5.02	5.458	801	795	793

Table 2. Concentration and Free volume at Different Temperatures for NNDMF+1 Butanol+n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Free Volume(V_f) m^3/mol	303 K	4.186	4.191	4.189	4.179	4.016	3.993	3.996	3.962	3.941	3.863
	308 K	3.706	3.676	3.691	3.699	3.658	3.639	3.591	3.595	3.575	3.569
	313 K	3.276	3.260	3.236	3.216	3.183	3.179	3.158	3.136	3.108	3.094

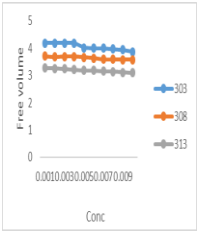


Table 3. Concentration and Cohesive Energy at Different Temperatures for NNDMF+1 Butanol+n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Cohesive Energy Kj/mol	303 K	33.882	35.019	35.019	35.040	35.503	35.527	35.53	35.632	35.745	35.965
	308 K	35.125	35.732	36.825	36.223	36.026	37.094	37.753	38.299	38.527	38.659
	313 K	37.425	38.722	38.828	38.923	39.066	39.098	39.193	39.299	39.427	39.490

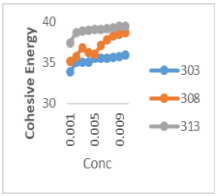


Table 4. Concentration and Gibbs Free Energy at Different Temperatures for NNDMF+1 Butanol+ n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Gibbs free energy (ΔG) Kj/mol	303 K	-15.08	-15.08	-15.07	-15.07	-15.00	-15.00	-15.00	-14.99	-14.97	-14.94
	308 K	-14.70	-14.7	-14.70	-14.69	-14.67	-14.67	-14.65	-14.65	-14.64	-14.64
	313 K	-14.45	-14.43	-14.42	-14.41	-14.39	-14.38	-14.37	-14.36	-14.35	-14.34

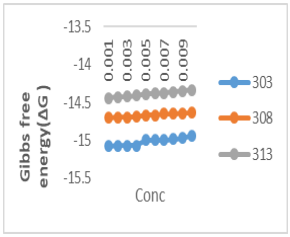


Table 5. Concentration and Free Length at Different Temperatures for NNDMF+1 Butanol+n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Free Length (L_f) (m)x 10^{-1}	303 K	6.71	6.66	6.66	6.65	6.65	6.64	6.64	6.63	6.63	6.63
	308 K	6.86	6.79	6.79	6.8	6.79	6.79	6.78	6.77	6.76	6.76
	313 K	6.93	6.87	6.87	6.87	6.87	6.86	6.86	6.86	6.85	6.85

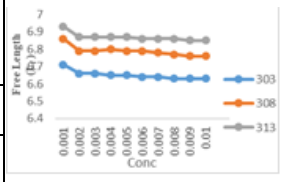


Table 6. Concentration and Adiabatic Compressibilityat Different Temperatures for NNDMF+1 Butanol+n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Adiabatic Compressibility (β) $N^{-1}m^2x10^{-}$	303 K	1.14	1.15	1.15	1.14	1.14	1.14	1.14	1.14	1.14	1.1
	308 K	1.19	1.19	1.19	1.19	1.19	1.19	1.19	1.19	1.18	1.1
	313 K	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.21	1.2

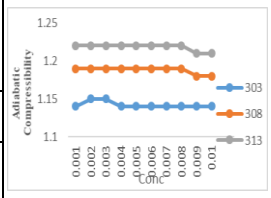


Table 7. Concentration and Internal Pressure at Different Temperatures for NNDMF+1 Butanol+n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Internal Pressure (Nm^{-2}) $x10^{+8}$	303 K	2.67	3.332	3.332	3.334	3.37	3.39	3.387	3.4	3.401	3.422
	308 K	2.904	3.636	3.646	3.65	3.663	3.672	3.682	3.694	3.705	3.708
	313 K	2.917	3.653	3.663	3.672	3.682	3.685	3.694	3.704	3.716	3.722

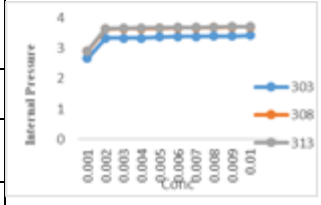


Table 8. Concentration and Relaxation Time at Different Temperatures for NNDMF+1 Butanol+n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Relaxation Time (τ)(s)x 10^{-16}	303 K	6.737	6.747	6.754	6.754	6.931	6.929	6.944	6.962	7.002	7.091
	308 K	7.719	7.73	7.741	7.752	7.81	7.821	7.861	7.875	7.899	7.915
	313 K	8.479	8.518	8.552	8.595	8.662	8.667	8.7	8.744	8.794	8.822

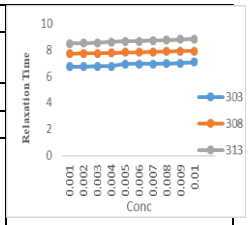


Table 9. Concentration and Absorption Coefficient at Different Temperatures for NNDMF+1 Butanol+ n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Absorption Coefficient x10^{-17}	303 K	1.27	1.27	1.28	1.27	1.31	1.31	1.31	1.31	1.32	1.33
	308 K	1.48	1.48	1.49	1.49	1.5	1.51	1.51	1.51	1.51	1.51
	313 K	1.65	1.65	1.66	1.67	1.68	1.68	1.68	1.69	1.7	1.71

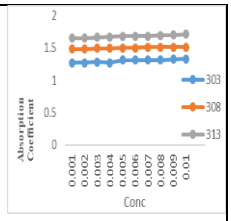
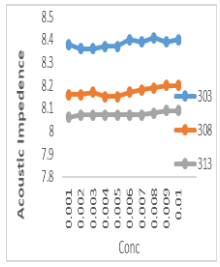


Table 10. Concentration and Acoustic Impedence at Different Temperatures for NNDMF+1 Butanol+ n Hexane

S.No.		1	2	3	4	5	6	7	8	9	10
Conc. (M)		0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
Acoustic Impedence (x10^{+5})	303 K	8.38	8.36	8.36	8.37	8.37	8.4	8.39	8.41	8.39	8.4
	308 K	8.16	8.16	8.17	8.15	8.15	8.17	8.18	8.19	8.20	8.20
	313 K	8.06	8.07	8.07	8.07	8.07	8.07	8.07	8.08	8.09	8.09



4. CONCLUSION

The following conclusions are drawn:

1. The increase in temperature due to thermal agitation, resulting in a decrease in ultrasonic velocity. An increase in viscosity with increase in concentration suggests that molecular interactions are increasing in thickness of the liquid mixture and molecular size and shape of the elements that play an equally important role.
2. The adiabatic compressibility suggests that the lack of interaction between unlike molecules that have the minimum declarations.
3. The weak interactions accounted for positive higher values, while the dipole-dipole, dipole-induced dipole, charge transfer and hydrogen bonding are unlike the system of negative ones. From the magnitude of velocity, there is molecular interactions in the mixture, which are linked to the C=O group of NNDMF resulting in a weak link between them.
4. The interactions are due to dipole-dipole interaction and the polar nature of different molecular entities in the mixture.

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Conflict of Interest

None of the authors have any conflicts of interest to declare.

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