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ULTRASONIC STUDY OF MOLECULAR INTERACTIONS IN BINARY LIQUID MIXTURES OF ACETYLACETONE WITH n-HEXANE AND n-HEPTANE USING EXCESS ACOUSTIC PARAMETERS

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ABSTRACT

The ultrasonic velocity (u), density (ρ) have been measured at 2MHz frequency and temperature 303K for binary systems Acetylacetone with n-Hexane and n-Heptane. From the measured parameters excess parameters such as excess adiabatic compressibility (β^E), excess intermolecular free length $\left(L_f^E\right)$, excess acoustic impedance (Z^E) , excess interaction parameter (χ^E) and excess molar volume $\left(M_f^E\right)$ have been calculated and represented as functions of molar volume of Acetylacetone. The values of u^E, Z^E and χ^E are negative where as β^E, L_f^E and V_m^E are positive for both systems, represents there is no much interaction between unlike molecules.

KEYWORD: Acetylacetone, n-Hexane, n-Heptane, excess acoustic compressibility, excess acoustic impedance, excess free length.

INTRODUCTION

Literature survey on ultrasonic studies shows that still it is one of the potential tool in finding the intermolecular interactions in binary liquid mixtures. In this paper author made an attempt to explain intermolecular interactions in binary liquid mixtures using excess thermodynamic parameters derived from experimentally measured ultrasonic velocity (u) and density (ρ). In phase with ongoing research work and usage of n-Hexane, n-Heptane and particularly Acetylacetone in the production of anticorrosion agents in industries stimulated us to study binary systems (a) Acetylacetone + n-Hexane (b) Acetylacetone + n-Heptane at 2 MHz and at constant temperature 303 K using ultrasound techniques [1-5]. From the experimental data excess parameters such as excess adiabatic compressibility (β^E), excess intermolecular free length $\left(L_f^E\right)$, excess acoustic impedance (Z^E), excess interaction parameter (χ^E) and excess molar volume $\left(M_f^E\right)$ have been calculated and represented as functions of molar volume of Acetylacetone.

MATERIALS AND METHODS

The chemicals Acetylacetone, n-Hexane and n-Heptane used were of HPLC grade and obtained from S.D. Fine Chemicals Limited (SDFCL). The purity of the sample was checked by measuring density of pure liquids using specific gravity bottle. Weights are measured using a single pan analytical balance with precession 1 mg and their values are compared with the literature values.[6-8] All 9 mole fractions are prepared by mixing appropriate volumes of the liquid components of Acetylacetone + n-Hexane and Acetylacetone + n-Heptane and preserved in the air tight volumetric flasks of 25ml capacity at room temperature. After mixing, the volumetric flasks are undisturbed in order to attain the thermal equilibrium.

MEASUREMENT OF ULTRASOUND SPEED

The speed of sound is measured using ultrasonic interferometer (Model M-81) supplied by Mittal Enterprises, New Delhi. It consists of (a) high frequency generator and (b) measuring cell .The ultrasonic interferometer has an accuracy of ±0.5 m/s. The temperature of the solution was controlled by circulating water through the jacket of doubled walled cell using temperature controlled constant water bath having precession ±0.1^0 C. A quartz crystal which generates a particular frequency is fixed at the bottom of the cell. A fine digital micrometer screw is with least count (LC) ±0.001 mm is provided at the top of the plunger.

The principle involved in measuring ultrasonic speed is when ultrasonic waves propagate through the binary mixture, stationary waves will setup. The measured distance between two consecutive minima's represents λ/2. Ultrasonic velocity is measured for known frequency using the formula $u = 2f \times (\lambda/2)$.

Table1: Experimental and Literature Values of Density (ρ) & Ultrasonic velocity of Pure Liquids at 303K

Liquids	Density (ρ) kgm^{-3}		Ultrasonic velocity (u) ms^{-1}	
	Experimental	Literature	Experimental	Literature
Acetylacetone	973.1579	966.1 [6]	1272	1293
n-Hexane	656.0526	650.1 [7]	1056	1058
n-Heptane	681.2281	675.44 [8]	1100	945.56 [8]

Table 2: Experimental parameters Density (ρ), velocity (U) for Binary mixtures Acetylacetone + n-Hexane are listed at f = 2 MHz and T = 303 K

Mole fraction Of Acetylacetone X_1	Mole fraction Of n-Hexane X_2	ρ_m kgm^{-3}	U ms^{-1}
1	0	973.1579	1272
0.921972	0.078028	940.3509	1244
0.840039	0.159961	907.2807	1208
0.7539	0.2461	872.6316	1188
0.663223	0.336777	842.0175	1156
0.567639	0.432361	812.2807	1136
0.466739	0.533261	778.4211	1108
0.360067	0.639933	749.2982	1088
0.247113	0.752887	718.7719	1072
0.127305	0.872695	687.4561	1048
0	1	656.0526	1056

Table 3: Derived parameters - Excess Density (ρ^E), Excess velocity (U^E) for Binary mixtures Acetylacetone + n-Hexane are listed at f = 2 MHz and T = 303 K

Mole fraction Of Acetylacetone X_1	Mole fraction Of n-Hexane X_2	ρ^E kgm^{-3}	U^E ms^{-1}
1	0	0.0000	0.0000
0.921972	0.078028	-8.0640	-11.1460
0.840039	0.159961	-15.1527	-29.4484
0.7539	0.2461	-22.4867	-30.8424
0.663223	0.336777	-24.3465	-43.2561
0.567639	0.432361	-23.7732	-42.6100
0.466739	0.533261	-25.6370	-48.8156
0.360067	0.639933	-20.9335	-45.7745
0.247113	0.752887	-15.6415	-37.3764
0.127305	0.872695	-8.9656	-35.4979
0	1	0.0000	0.0000

Table 4: Excess Adiabatic compressibility (β^E), Excess Inter molecular free length (L_f^E), Excess Acoustic Impedance (Z^E), Excess Interactivity parameter (χ^E) and Excess Molar Volume (V_m^E) for Binary mixtures Acetylacetone + n-Hexane are listed at f = 2 MHz and T = 303 K

Mole fraction Of Acetylacetone X_1	$\beta^E \times 10^{-10}$ $N^{-1}m^2$	$L_f^E \times 10^{-6}$ m	$Z^E \times 10^6$ $kgm^{-2}s^{-1}$	χ^E	$V_m^E \times 10^{-4}$ m^3
1	0.0000	0.0000	0.0000	0.0000	0.0000
0.921972	-0.0502	1.9603	-2.5530	-0.5759	2.1059
0.840039	0.0315	8.2771	-5.4673	-1.4445	4.5712
0.7539	-0.0323	8.2398	-6.7030	-1.5294	9.1207
0.663223	0.0717	13.4084	-8.0919	-2.0721	8.5702
0.567639	0.0248	12.3729	-7.9441	-2.0311	6.4339
0.466739	0.2108	18.0646	-8.4704	-2.2542	10.0156
0.360067	0.2403	17.5080	-7.3815	-2.0749	6.0685
0.247113	0.2460	15.1794	-5.6961	-1.6646	3.6833
0.127305	0.5071	19.0860	-4.1727	-1.4918	2.0669
0	0.0000	0.0000	0.0000	0.0000	0.0000

Table 5: Experimental parameters Density (ρ), velocity (U) for Binary mixtures Acetylacetone + n-Heptane are listed at f = 2 MHz and T = 303 K

Mole fraction Of Acetylacetone X_1	Mole fraction Of n-Heptane X_2	ρ_m kgm^{-3}	U ms^{-1}
1	0	973.1579	1272
0.929347	0.070653	941.9298	1248
0.853932	0.146068	912.3684	1216
0.773255	0.226745	883.7719	1196
0.686746	0.313254	852.3684	1168
0.593749	0.406251	822.8947	1156
0.493505	0.506495	796.2281	1132
0.385134	0.614866	767.193	1124
0.267605	0.732395	737.6316	1116
0.139705	0.860295	711.5789	1112
0	1	681.2281	1100

Table 6: Derived parameters - Excess Density (ρ^E), Excess velocity (U^E) for Binary mixtures Acetylacetone + n-Heptane are listed at f = 2 MHz and T = 303 K

Mole fraction Of Acetylacetone X_1	Mole fraction Of n-Heptane X_2	ρ^E kgm^{-3}	U^E ms^{-1}
1	0	0.0000	0
0.929347	0.070653	-10.6025	-11.847761
0.853932	0.146068	-18.1478	-30.876281

0.773255	0.226745	-23.1923	-36.999826
0.686746	0.313254	-29.3412	-50.120268
0.593749	0.406251	-31.6663	-46.124761
0.493505	0.506495	-29.0688	-52.882869
0.385134	0.614866	-26.4671	-42.243008
0.267605	0.732395	-21.7182	-30.027974
0.139705	0.860295	-10.4332	-12.029292
0	1	0.0000	0

Table 7: Excess Adiabatic compressibility (β^E), Excess Inter molecular free length (L_f^E), Excess Acoustic Impedance (Z^E), Excess Interactivity parameter (χ^E) and Excess Molar Volume (V_m^E) for Binary mixtures Acetylacetone + n-Heptane are listed at f = 2 MHz and T = 303 K

Mole fraction Of Acetylacetone X_1	$\beta^E \times 10^{-10}$ $N^{-1}m^2$	$L_f^E \times 10^{-6}$ M	$Z^E \times 10^6$ $kgm^{-2}s^{-1}$	χ^E	$V_m^E \times 10^{-4}$ m^3
1	0.0000	0.0000	0.0000	0.0000	0.0000
0.929347	0.0569	4.7021	-2.7814	-0.5626	2.9356
0.853932	0.2171	12.8254	-5.7062	-1.4172	4.1046
0.773255	0.2486	15.3711	-7.0099	-1.6895	4.0252
0.686746	0.4379	22.9851	-8.9264	-2.2387	7.6097
0.593749	0.3943	21.6336	-8.8134	-2.0600	8.6714
0.493505	0.5221	25.4826	-8.9101	-2.3091	5.2200
0.385134	0.4119	20.7175	-7.5166	-1.8440	5.0345
0.267605	0.3003	15.3307	-5.6880	-1.3103	5.5334
0.139705	0.0408	4.7020	-2.6322	-0.5413	-1.1374
0	0.0000	0.0000	0.0000	0.0000	0.0000

RESULTS AND DISCUSSIONS

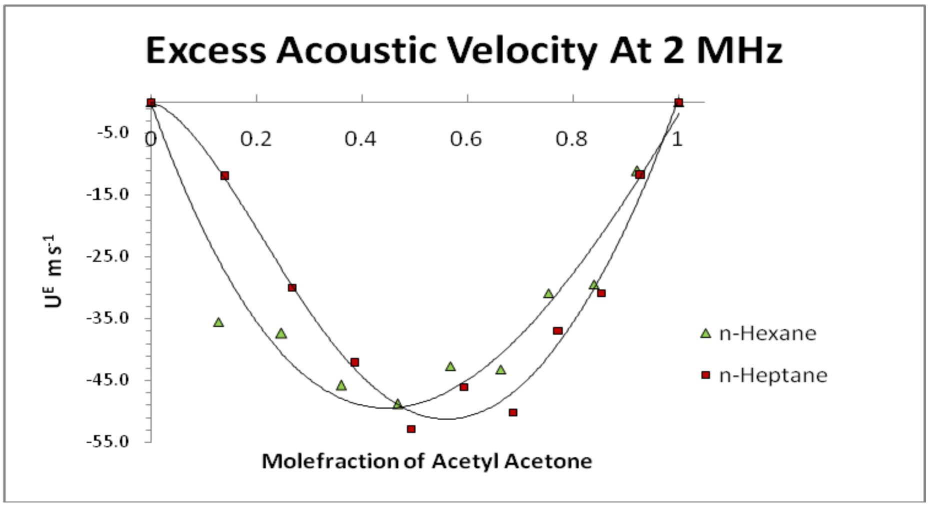

Fig. 1 Variation of excess acoustic velocity with mole fraction of Acetylacetone

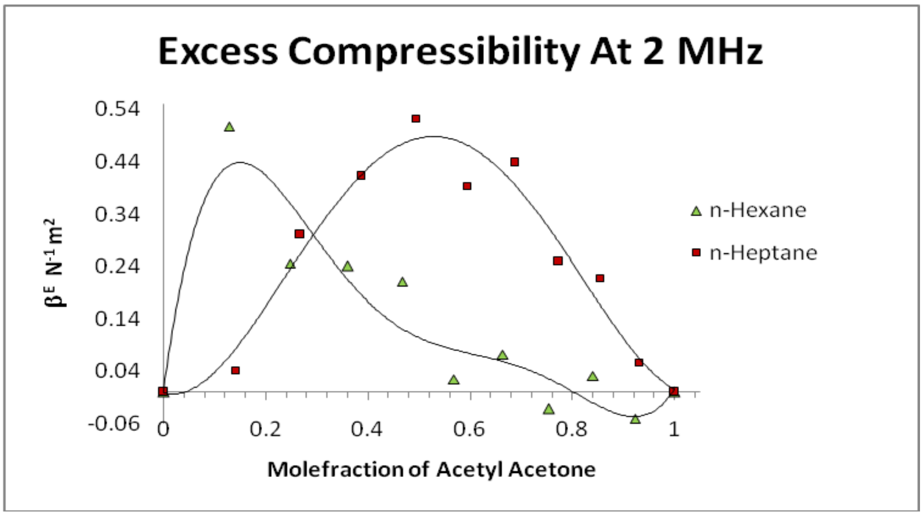

Fig. 2 Variation of excess compressibility with mole fraction of actylacetone

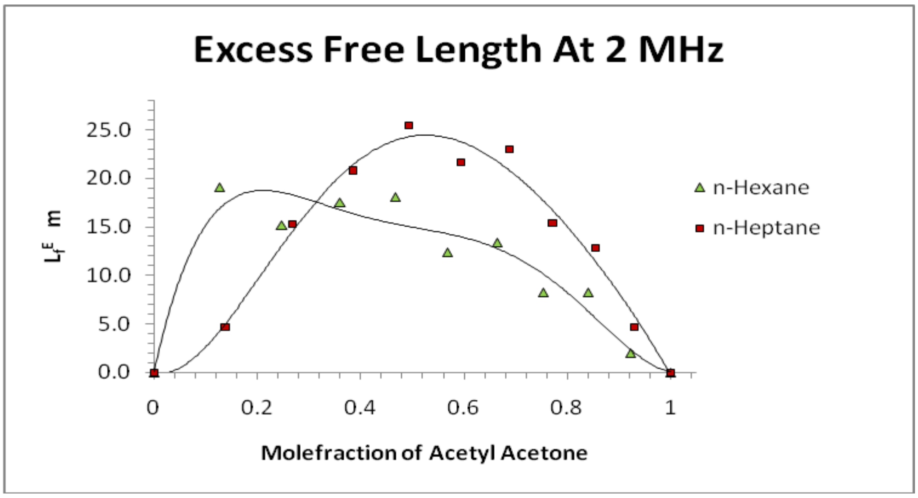

Fig. 3 Variation of excess free length with mole fraction of Acetylacetone

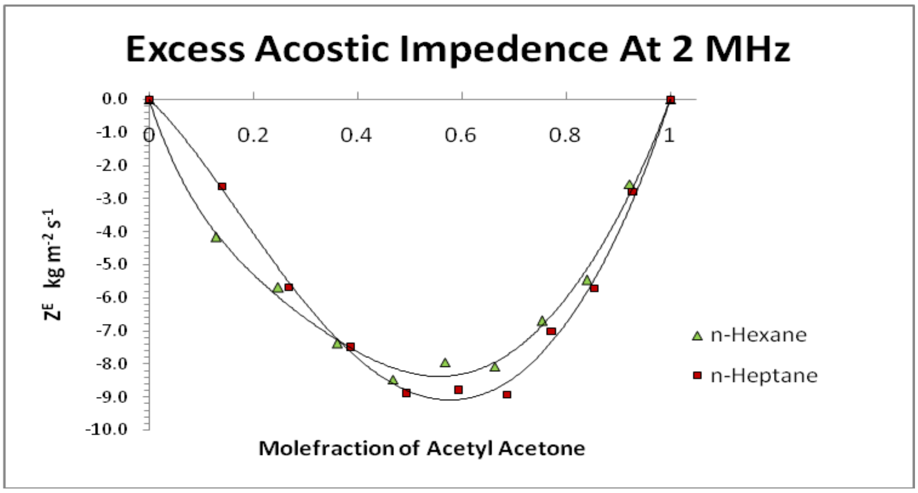

Fig. 4 Variation of excess acostic impedence with mole fraction of acetylacetone

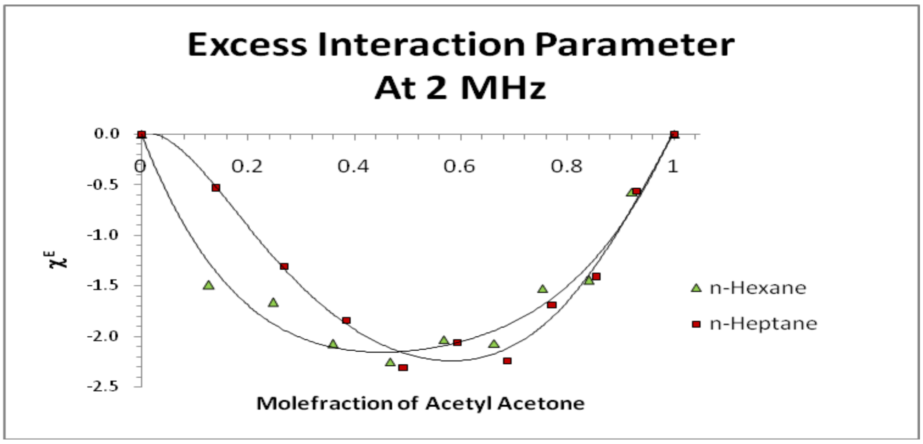

Fig. 5 Variation of excess interaction parameter with mole fraction of Acetylacetone

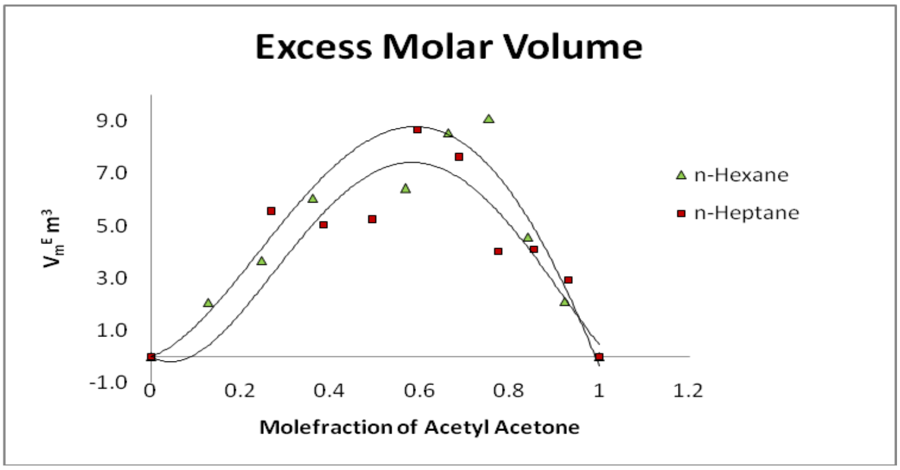

Fig. 6 Variation of molar volume with mole fraction of anisole

Excess Acoustic Velocity

In fig.1 the trend in excess acoustic velocity (u^E) is negative for entire mole fractions of Acetylacetone. It suggests the presence weak intermolecular interactions exist within the component of molecules. The excess negative velocity is less for n-Hexane compare to n-Heptane. This shows that as chain length decreases approach of unlike molecules increases.

Excess Adiabatic Compressibility(β^E) and Excess Free length L_f^E

The variation of excess adiabatic compressibility's and free length in fig.2 and fig.3 are found to be positive for all mole fractions of Acetylacetone indicates the weak interactions between Acetylacetone and n-Hexane / n-Heptane. This is due to the breaking of hydrogen bond.[9-14] Excess compressibility is positive means β_{mix} is more than pure liquids (1) and (2). It shows that liquid mixture is highly compressed and it is possible only when unlike molecules are less tightly bound or interaction is less. Positive value of L_f^E reflects weak interaction and it is due to the disassociation of molecules.

Excess Acoustic Impedance(Z^E)

Acoustic impedance (Z^E) is the opposition offered by the medium for the propagation of sound energy. In fig.4 negative deviation of excess acoustic impedance is maximum when solute and solvent are in almost equal ratio, signifies strongly there is no polar and non-polar molecular interactions. However the magnitude of molecular association increases as component of Acetylacetone (polar molecules) increases. From the figure it shows that weak interactions exist in the mixtures which are in the order n-Heptane > n-Hexane. As chain length decreases association between unlike molecules are more due to easier approach of unlike molecules.[15]

Excess Interaction parameter(χ^E)

In fig.5 from the plot of graph for both systems (χ^E) decreases negatively and there is a negative peak when mole fractions of solute and solvent are almost 50%. However it is less negative for n-Hexane shows that slightly association between solute and solvent is better than n-Heptane. Negative peak indicates the absence any complex formation but interaction is maximum in rich region of Acetylacetone.

Excess Molar Volume $\left(V_m^E\right)$

In fig.6 the positive deviation in excess molar volume for both systems indicates weak interactions between component of molecules. [16] Probably it is due to two reasons. (i) Breaking of hydrogen bonds chain length is prominent (ii) Molar volume of Acetylacetone (11.69×10^{-6}), n-Hexane (11.63×10^{-6}) and n-Heptane (1181×10^{-6}) are almost same, so that component molecules are not packed well. This results into increase in volume, hence $\left(V_m^E\right)$ is positive for entire range of mole fraction.

CONCLUSION

The ultrasonic technique is found to be most powerful tool in characterising physico chemical behavior of binary mixtures. From the experimental data variation of acoustic parameters with mole fraction indicate the presence of weak interactions for entire range of *mole fraction* of Acetylacetone. Actually interaction should increase with chain length. But on the contrary we found that less interaction or association for n-Heptane compare to n-Hexane. Probably this is due to as chain length decreases approach of unlike molecules are becoming stronger. However it is observed that in all acoustic parameters there is no much significant variations between n-Hexane and n-Heptane.

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