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Acoustic, Thermodynamic and Viscosity Studies of Dimethyl Carbonate Binary Mixes with Higher Alkanols

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ABSTRACT

The measurements of speed of viscosity (η) ultrasonic sound (U) and density (ρ) for the Dimethyl Carbonate binary mixes with higher alkanols at four distinct temperatures (303.15-318.15K) spanning the whole composition range. Excess values of molar volume, intermolecular free length, and acoustic impedance values, as well as deviations in adiabatic compressibility and viscosity, were computed. The equation of Redlich-Kister polynomial was fitted to the calculated excess values in order to determine binary constants and the standard deviation (σ).

Keywords: Dimethyl carbonate, Densities, Speed of sound, Viscosity compressibilities, Molar volumes, Inter molecular free lengths, Acoustic impedance.

INTRODUCTION

Compared to pure liquids, liquid mixtures are utilized in a wide range of sectors because they give a diverse range of solvents with the necessary properties[1,2,3]. The physico-chemical studies of binary liquid mixes give a solid tool that has tremendously benefited both theoretical and practical areas of study and chemical engineering by increasing our understanding of the interactions' strength between constituent molecules and also the nature of interactions. The behaviour of mixes as a function of composition, temperature, and other factors can be theoretically explained using data, whilst experimentally determined parameters can be changed realistically to offer the desired properties[4,5,6,7].

It is for this reason that the intermolecular interactions' investigation that occur in binary liquid mixtures is very significant. The fundamental mechanisms are still comparatively little known at a precise molecular level in the case of a binary mixtures of fragrance molecules. In order to study the thermodynamic properties and the molecular interactions of Dimethyl Carbonate with higher alkanols which is the extension of our recent study DMC with salicylates same parameters were measured at same temperatures as in our previous work.

DMC is an aprotic, polar solvent having a dipole moment of 0.90 D. DMC mainly used as an intermediate in synthesis of various polymers and also used in electrolytes for lithium-ion batteries, which are expected to play a major role in energy storage, used in biodiesel production, in construction material such as paints, cleaning and degreasing processes. Alkanols are used in the medicine and perfumery industry as solvent, as alternative fuel for internal combustions etc. Thus, the growing demand of the alkanols and DMC in various applications emphasizes its need to study the thermodynamic properties of these liquids and their binary mixtures at different temperatures.

EXPERIMENTAL

Velocity Measurements

The ultrasonic velocity can be computed using the formula $U=\lambda f$. The generator used in the study has a frequency of 2 MHz. We should record the number of times the anode current was at its maximum while adjusting the micrometer screw for n peaks.

$$d = n\lambda/2$$

It is simple to calculate the speed in meters per second by multiplying the reflector's displace-ment by 20 peaks by 100.The accuracy of the velocity primarily depends on the quality of thedistance measurement because the distance 'd' may be measured with a micrometer to an accuracy of 0.01 mm or greater. The acceleration measurement has a precision of +0.02%

Density Measurements

The density (ρ) was measured for pure liquids and all liquid mixes at different temperatures between 303.15K and 318.15K with a 5K interval are measured in the current study using a specific gravity bottle with a 5 mL volume. The density of the liquids was one of the criteria used to determine their purity. The specific gravity bottle was left in the thermostat for fifteen minutes in order to reach thermal equilibrium. They are removed from the thermostat and weighed when they are at room temperature. The density readings have a margin of error of 0.5 mg.

Viscosity Measurements

A 0.55mm diameter Ubbelohde capillary viscometer calibrated with double-distilled water was used to measure the viscosity at 303.15, 308.15, 313.15, and 318.15K. Pure water is used to calibrate the viscometer, and to reduce temperature fluctuations, the liquid is left to stand in a thermostatic water bath for around 30 minutes. The viscosity readings have a 0.005 mPas precision.

Theoretical Considerations

Molar volume

$$V = M/\rho \quad (1)$$

Excess Volume (V^E)

$$V^E = V - (V_1X_1+V_2X_2) \quad (2)$$

Where X_1 indicates the mole fractions of common compound and X_2 indicates the mole fraction of sub compound and the molar volumes are V_1 & V_2 respectively.

Adiabatic Compressibility (βad)

$$\beta_{ad} = 1/\rho U^2 \quad (3)$$

Deviation in Adiabatic compressibility ($\Delta\beta_{ad}$)

$$\Delta\beta_{ad} = \beta_{ad} - (\beta_{ad1}X_1 + \beta_{ad2}X_2) \quad (4)$$

Where pure liquids' adiabatic compres-sibilities are indicated as β_{ad1} and β_{ad2}.

Intermolecular free length (Lf)

$$L_f = K (\beta_{ad})^{1/2} \quad (5)$$

Jacobson constant is indicated as K.

Excess Intermolecular free length (Lf^E)

$$L_f^E = L_f - (L_{f1}X_1 + L_{f2}X_2) \quad (6)$$

Pure liquids' intermolecular free length are L_{f1} and L_{f2} respectively

Deviation in Viscosity ($\Delta\eta$)

$$\Delta\eta = \eta_{mix} - (X_1\eta_1 + X_2\eta_2) \quad (7)$$

The liquid mixture and the pure liquids' viscosities are indicated as η_{mix}, η_1 and η_2 are respectively.

Acoustic impedance (Z)

$$Z = U\rho \quad (8)$$

Excess Acoustic impedance (Z^E)

$$Z^E = Z_{mix} - (X_1Z_1+X_2Z_2) \quad (9)$$

The excess/deviation values of $\Delta\beta_{ad}$, V^E, $\Delta\eta$, L_f^E, Z^E were fitted to the Redlich–Kister type polynomial[9]

$$Y^E = X(1-X)\sum_{i=1}^{n} A_i(1-2X)^{i-1} \quad (10)$$

The coefficients of Ai and standard deviation (σ) are given in Tables 3 using the following relation

$$\sigma Y^E = \sum\left[\frac{\left[Y^E_{exp} - Y^E_{cal}\right]^2}{m-n}\right]^{1/2} \quad (11)$$

Here the experimental data points are denoted by m number and number of coefficients is indicated as n (n = 5 in the present calculation).

Purification of solvents

It is essential to make sure the substances used are as pure as possible, as the purity of the liquid impacts the accuracy and precision of the results. The type and functional groups of the compounds were taken into consideration when developing various purification techniques, which are described in detail in the literature[9-11].

Table 1: Literature Data in comparison with experimental data[12-15] at 303.15K

Liquid	(ρ) gm/cc		(U)m/s		(η)cP	
	Experimental	Literature	Experimental	Literature	Experimental	Literature
DMC	1.0562	1.0567112	1175.3	117712	0.549	0.54912
1- Hexanol	0.8135	0.810213	1289.5	1289.513	3.7655	3.513013
1- Heptanol	0.815714	0.815514	1313.2	1312.014	5.0500	5.049014
1-Octanol	0.8199	0.818214	1333.1	1340.014	6.4050	6.402014

All of the organic liquids that are offered are of the highest quality. The liquids require around five to six hours to establish temperature equilibrium after distillation, mixing with a burette, and use in an experiment.

The findings of comparing the experimental values with data from the literature are shown in Table 1.

RESULTS

Table 2 displays the experimental results for ρ, η and U for the three binary mixes (Dimethyl Carbonate + higher alkanols) at four temperatures. The experimentally recorded values fluctuate nonlinearly with the mole fraction of Dimethyl Carbonate, indicating this specific interaction between different molecules.

Table 2 shows that as the temperature of a binary liquid rises, its ultrasonic wave velocity decreases at all studied temperatures over the whole mole fraction range. The bonds between molecules may become more easily broken at higher temperatures. When heat is applied to a binary mixture, the distance between molecules increases, allowing sound waves to travel further than they would in their pure solvents. As the temperature of a binary mixture rises, so does the rate at which ultrasonic waves travel through it.

According to Table 3, the binary liquid combination loses density and viscosity as its temperature rises. Particularly sensitive to inter-molecular interactions in liquid mixtures are excess characteristics such molar volume (V^E), intermolecular freelength (L_f^E) and acoustic impedance (Z^E) and viscosity and adiabatic compressibility deviations ($\Delta\eta$ & $\Delta\beta_{ad}$), which can be used to characterize the effect of interaction.[15]

Several effects that might act in the same or opposing directions determine the sign and amount of excess functions that arise when two components are mixed[16-18]. The excess properties are highly responsive to variations in the mixture's molecule size as well as the shape. A variety of causes contribute to excess values. Van der Waal forces and other non-specific interactions are examples of physical contributions. Specific interactions between the component molecules, including charge transfer complexes, H-bonding, and strong dipole–dipole interactions, make up the chemical contributions. Molecules of small size in one component may fit into the spaces of other component's bigger molecules in a favorable or unfavorable way, which results in structural contributions[18,19].

Table 2: Ultrasonic velocity (U)m/s, density (ρ) Kg/m³, viscosity(η)cp for Dimethyl Carbonate with three higher alkanols binary mixtures under study

X_1	(U)m/s	(ρ) gm/cc	(η)cP	(U)m/s	(ρ) gm/cc	(η)cP	(U)m/s	(ρ)gm/cc	(η)cP	(U)m/s	(ρ) gm/cc	(η)cP
		303.15K			308.15K			313.15K			318.15K	
						DMC+1-Hexanol						
0	1289.5	0.8135	3.7655	1280.0	0.8080		1256.5		3.0350	1236.5	0.8001	2.9346
0.1406	1288.0	0.8409	4.146	1282.0	0.8359	3.3520	1263.0	0.8042	3.2790	1244.2	0.8283	3.1020
0.2691	1287.2	0.8672	4.2967	1280.0	0.8621	3.6917	1262.5	0.8321	3.5299	1246.3	0.854	3.3245
0.3869	1285.6	0.8931	4.3568	1278.0	0.8878	3.8402	1261.6	0.8581	3.5209	1243.9	0.8793	3.3641
0.4954	1282.3	0.9184	4.2936	1273.5	0.9132	3.9070	1253.8	0.8834	3.4951	1235.3	0.9041	3.3257
0.5956	1271.2	0.9432	4.1356	1259.0	0.9380	3.8609	1238.5	0.9086	3.3840	1220.1	0.9281	3.2155
0.6884	1252.5	0.9675	3.5825	1239.0	0.9621	3.7310	1220.1	0.9330	2.9489	1202.6	0.9520	2.8050
0.7746	1233.6	0.9910	2.8906	1218.0	0.9859	3.2418	1200.6	0.9570	2.4016	1182.8	0.9755	2.2930
0.8549	1211.8	1.0139	2.2901	1195.9	1.0089	2.6390	1180.5	0.9807	1.7995	1161.1	0.9980	1.5856
0.9298	1192.0	1.0360	1.5470	1175.0	1.0309	2.0125	1157.6	1.0032	1.1570	1138.2	1.0191	1.0250
1	1175.3	1.0566	0.5490	1153.7	1.0507	1.2954	1135	1.0247	0.4860	1113	1.0367	0.4730
					0.518		1.043					
						DMC+1- Heptanol						
0	1313.2	0.8157	5.0500	1297.0	0.8114	4.3410	1278.0	0.8077	4.009	0.7859	0.7859	3.6405
0.1565	1307.0	0.8420	4.9958	1295.0	0.8382	4.3025	1280.0	0.8345	3.896	0.8138	0.8138	3.4600
0.2945	1303.0	0.8679	4.8980	1291.4	0.8640	4.2590	1276.5	0.8599	3.8286	0.8405	0.8405	3.4306
0.4172	1299.0	0.8935	4.7800	1286.5	0.8893	4.1885	1273.3	0.8849	3.7876	0.8669	0.8669	3.4822
0.5268	1292.3	0.9185	4.5890	1281.2	0.9143	4.0656	1263.0	0.9097	3.674	0.8930	0.8930	3.3935
0.6255	1280.0	0.9432	4.2500	1264.3	0.9387	3.7881	1245.5	0.9338	3.4651	0.9185	0.9185	3.2140
0.7147	1259.0	0.9673	3.5546	1243.1	0.9625	3.1570	1225.0	0.9575	2.8924	0.9440	0.9440	2.6919
0.7958	1235.5	0.9904	2.8460	1220.0	0.9861	2.5406	1203.2	0.9810	2.3004	0.9691	0.9691	2.0004
0.8698	1212.0	1.0132	2.0954	1196.1	1.0087	1.7496	1181.2	1.0030	1.4860	0.9931	0.9931	1.3056
0.9376	1192.1	1.0349	1.2956	1173.0	1.0305	1.0578	1157.7	1.0230	0.8709	1.0160	1.0160	0.7810
1.0000	1175.3	1.0562	0.5490	1153.7	1.0507	0.5180	1135.0	1.0433	0.4860	1.0367	1.0367	0.4730
0.0000	1333.1	0.8199	6.4050	1315.7	0.8148	5.4200	1298.9	0.8113	4.6280	1284.9	0.8001	3.8580
0.1718	1322.0	0.8450	5.9569	1308.1	0.8404	5.0389	1295.7	0.8371	4.2780	1282.2	0.8262	3.5807
0.3183	1314.8	0.8704	5.5998	1301.5	0.8657	4.8034	1290.2	0.8621	4.1210	1278.0	0.8517	3.4860
0.4446	1307.7	0.8955	5.2005	1295.1	0.8906	4.5057	1283.5	0.8869	3.9547	1269.5	0.8768	3.3887
0.5546	1299.4	0.9202	4.8596	1287.7	0.9152	4.2783	1270.4	0.9113	3.7801	1257.4	0.9015	3.2960
0.6513	1285.0	0.9446	4.5049	1268.5	0.9395	3.9857	1252.0	0.9350	3.5471	1235.5	0.9259	3.1879
0.7369	1261.9	0.9680	3.6589	1245.6	0.9630	3.3021	1228.5	0.9584	2.9541	1212.2	0.9499	2.5200
0.8134	1235.8	0.9910	2.9059	1220.7	0.9857	2.5896	1205.8	0.9814	2.2578	1188.4	0.9735	1.9570
0.8819	1210.6	1.0132	2.0490	1194.5	1.0075	1.7958	1182.0	1.0028	1.6087	1163.7	0.9959	1.3500
0.9438	1191.4	1.0345	1.2190	1172.8	1.0294	1.0560	1157.5	1.0225	0.9256	1137.4	1.0165	0.8179
1.0000	1175.3	1.0562	0.5490	1153.7	1.0507	0.5180	1135.0	1.0433	0.4860	1113.0	1.0367	0.4730

Table 3: Deviation/excess values [V^E, L_f^E, Z^E, $\Delta\eta$ & $\Delta\beta_{ad}$] for binary mixtures of Dimethyl Carbonate with three higher alkanols under study under study

DMC+1-Hexanol						DMC+1-Heptanol						DMC+1-Octanol					
X_1	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E	X_1	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E	X_1	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E
								303.15K									
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1406	-1.4813	-0.4419	-0.0171	0.8330	6.9570	0.1565	-1.1668	-0.3567	-0.0138	0.6500	0.0027	0.1718	-0.9005	-0.2440	-0.0108	0.5580	-0.0014
0.2691	-2.8737	-0.6741	-0.0336	1.3970	15.3648	0.2945	-2.4751	-0.5933	-0.0295	1.1740	0.0096	0.3183	-2.1379	-0.4798	-0.0258	1.0590	0.0041
0.3869	-4.0852	-0.8238	-0.0482	1.8360	24.5453	0.4172	-3.7005	-0.7499	-0.0444	1.6080	0.0185	0.4446	-3.2901	-0.6438	-0.0399	1.3990	0.0121
0.4954	-5.0292	-0.8834	-0.0599	2.1220	33.1622	0.5268	-4.5556	-0.8071	-0.0550	1.9100	0.0261	0.5546	-4.2113	-0.7149	-0.0513	1.7020	0.0203
0.5956	-5.0956	-0.8801	-0.0610	2.2860	35.1626	0.6255	-4.7855	-0.8201	-0.0579	2.0150	0.0297	0.6513	-4.4597	-0.7497	-0.0543	1.9140	0.0242
0.6884	-4.3159	-0.8253	-0.0517	2.0310	30.0562	0.7147	-4.0465	-0.7646	-0.0489	1.7210	0.0250	0.7369	-3.6898	-0.6659	-0.0448	1.5690	0.0192
0.7746	-3.4281	-0.6997	-0.0410	1.6170	24.1599	0.7958	-2.9162	-0.6216	-0.0352	1.3780	0.0170	0.8134	-2.4861	-0.5546	-0.0301	1.2640	0.0110
0.8549	-2.1334	-0.5333	-0.0255	1.2740	14.7781	0.8698	-1.6845	-0.4667	-0.0202	0.9600	0.0088	0.8819	-1.2124	-0.3853	-0.0146	0.8090	0.0028
0.9298	-0.9615	-0.3161	-0.0115	0.7720	6.6168	0.9376	-0.706	-0.2361	-0.0085	0.4660	0.0030	0.9438	-0.4425	-0.1617	-0.0053	0.3410	-0.0005
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
								308.15K									
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1406	-2.1817	-0.5292	-0.0251	0.7380	12.3597	0.1565	-1.8480	-0.4597	-0.0216	0.560	0.0081	0.1718	-1.4608	-0.3409	-0.0173	0.461	0.0032
0.2691	-3.6549	-0.7530	-0.0424	1.2510	21.3611	0.2945	-3.3444	-0.6931	-0.0393	1.0440	0.0163	0.3183	-2.8988	-0.5772	-0.0345	0.944	0.0101
0.3869	-5.0137	-0.8815	-0.0587	1.6520	31.5118	0.4172	-4.5886	-0.8195	-0.0543	1.4420	0.0250	0.4446	-4.2210	-0.6983	-0.0504	1.265	0.0190
0.4954	-6.0196	-0.9556	-0.0710	1.9130	40.5611	0.5268	-5.7056	-0.8872	-0.0679	1.7390	0.0348	0.5546	-5.3393	-0.7705	-0.064	1.577	0.0287
0.5956	-5.8743	-0.9474	-0.0694	2.0670	40.6535	0.6255	-5.5175	-0.8745	-0.0657	1.8380	0.0345	0.6513	-5.1444	-0.7891	-0.0616	1.758	0.0284
0.6884	-5.0543	-0.8768	-0.0597	1.8410	35.3027	0.7147	-4.7728	-0.7983	-0.0567	1.5480	0.0299	0.7369	-4.4177	-0.7194	-0.0527	1.495	0.0242
0.7746	-4.0430	-0.7788	-0.0477	1.4820	28.7465	0.7958	-3.7306	-0.7110	-0.0442	1.2420	0.0235	0.8134	-3.3079	-0.5726	-0.0393	1.157	0.0172
0.8549	-2.7933	-0.6177	-0.0329	1.0830	20.2430	0.8698	-2.4386	-0.5418	-0.0288	0.7340	0.0151	0.8819	-1.8674	-0.364	-0.0221	0.699	0.0078
0.9298	-1.5279	-0.3871	-0.0179	0.5790	11.5991	0.9376	-1.0874	-0.3234	-0.0128	0.3010	0.0066	0.9438	-0.8442	-0.1967	-0.0099	0.263	0.0030
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
								313.15K									
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1406	-2.8097	-0.5793	-0.0317	0.6020	16.0433	0.1565	-2.4446	-0.5152	-0.0281	0.4380	0.0121	0.1718	-2.1314	-0.4389	-0.0249	0.3620	0.0084
0.2691	-4.4764	-0.8185	-0.0510	1.1810	26.1519	0.2945	-4.0222	-0.7362	-0.0466	0.8570	0.0207	0.3183	-3.802	-0.6692	-0.0446	0.8110	0.0170
0.3869	-5.9535	-0.9365	-0.0685	1.4720	36.8189	0.4172	-5.5179	-0.8668	-0.0643	1.2480	0.0311	0.4446	-5.2118	-0.8287	-0.0613	1.1680	0.0266
0.4954	-6.5873	-1.0275	-0.0762	1.7230	42.6711	0.5268	-6.1543	-0.9514	-0.0720	1.5210	0.0367	0.5546	-5.8119	-0.9082	-0.0685	1.4490	0.0316
0.5956	-6.2894	-1.0140	-0.0729	1.8670	41.5995	0.6255	-5.8914	-0.9366	-0.0689	1.6600	0.0357	0.6513	-5.7036	-0.891	-0.0671	1.6170	0.0319
0.6884	-5.5725	-0.9666	-0.0646	1.6690	37.6708	0.7147	-5.2118	-0.8909	-0.0609	1.4010	0.0322	0.7369	-4.914	-0.8435	-0.0576	1.3780	0.0275

0.7746	-4.6469	-0.8854	-0.0538	1.3410	32.4359	0.7958	-4.2795	-0.8258	-0.0498	1.0950	0.0272	0.8134	-4.0772	-0.7627	-0.0476	0.9990	0.0236
0.8549	-3.5112	-0.7071	-0.0406	0.9440	25.3618	0.8698	-3.1258	-0.6294	-0.0363	0.5410	0.0204	0.8819	-2.8717	-0.5459	-0.0334	0.6340	0.0166
0.9298	-1.8856	-0.4607	-0.0217	0.4920	14.2425	0.9376	-1.5551	-0.2820	-0.0180	0.1650	0.0096	0.9438	-1.3294	-0.2041	-0.0154	0.2070	0.0067
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
318.15K																	
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
1406	-3.2143	-0.6622	-0.0357	0.5140	18.1263	0.1565	-2.9183	-0.5502	-0.0331	0.3150	0.0139	0.1718	-2.4545	-0.4540	-0.0281	0.3040	0.0097
0.2691	-5.3197	-0.8888	-0.0597	1.0520	30.7744	0.2945	-4.7988	-0.8012	-0.0547	0.7230	0.0238	0.3183	-4.5057	-0.7156	-0.0519	0.7050	0.0204
0.3869	-6.7394	-1.0334	-0.0762	1.3820	40.7387	0.4172	-6.2200	-0.9517	-0.0713	1.1630	0.0329	0.4446	-5.8998	-0.8662	-0.0682	1.0360	0.0291
0.4954	-7.3355	-1.0991	-0.0833	1.6110	45.9603	0.5268	-6.9860	-1.0293	-0.0803	1.4220	0.0390	0.5546	-6.7449	-0.9287	-0.0780	1.3150	0.0357
0.5956	-7.0554	-1.0673	-0.0803	1.7470	45.0524	0.6255	-6.7082	-1.0003	-0.0771	1.5550	0.0380	0.6513	-6.3600	-0.9410	-0.0734	1.5340	0.0340
0.6884	-6.4492	-1.0280	-0.0734	1.5650	42.3267	0.7147	-6.0663	-0.9667	-0.0696	1.3150	0.0352	0.7369	-5.6565	-0.9023	-0.0650	1.1570	0.0307
0.7746	-5.4719	-0.9535	-0.0622	1.2650	37.0921	0.7958	-5.0584	-0.8852	-0.0578	0.8810	0.0302	0.8134	-4.7307	-0.8244	-0.0541	0.8520	0.0266
0.8549	-4.112	-0.7945	-0.0466	0.7550	28.8518	0.8698	-3.7140	-0.6994	-0.0423	0.4200	0.0228	0.8819	-3.4650	-0.6399	-0.0395	0.4770	0.0200
0.9298	-2.3946	-0.5301	-0.0271	0.3790	17.6247	0.9376	-2.0099	-0.4303	-0.0227	0.1100	0.0128	0.9438	-1.7033	-0.3176	-0.0193	0.1550	0.0094
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 4: Redlich-Kister coefficients and standard deviations

T/K	303.15K					308.15K					313.15K					318.15K				
	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E	$\Delta\beta_{ad}$	V^E	L_f^E	$\Delta\eta$	Z^E
DMC+1-Hexanol																				
A_0	-19.947	166.055	-0.238	9.062	131.785	-23.568	-3.809	-0.278	166.055	158.267	-25.808	-4.025	-0.298	7.242	166.055	166.055	-4.305	-0.328	6.719	179.93
A_1	9.461	0.443	0.120	-4.083	-102.684	7.657	0.550	0.096	-40.454	-85.076	2.254	0.673	0.031	-3.718	-40.454	-40.454	0.208	0.026	-3.476	-34.629
A_2	14.537	-0.281	0.181	-9.48	-130.104	16.703	-0.459	0.206	-34.012	-149.212	3.938	-1.413	0.052	-5.001	-34.012	-34.012	-2.057	0.003	-2.936	1.9940
A_3	-11.573	0.101	-0.145	3.814	114.089	-8.615	-0.128	-0.107	-10.977	80.007	1.309	0.247	0.013	3.820	-10.977	-10.977	1.136	0.066	3.511	-51.203
A_4	-8.705	-1.165	-0.111	15.913	91.567	-20.303	-2.553	-0.247	65.291	196.836	-5.93	-2.302	-0.07	5.908	65.291	65.291	-2.563	-0.046	0.920	48.468
σ	0.0955	0.0061	0.0012	0.0902	0.8585	0.0777	0.0061	0.0009	0.9747	0.7224	0.1311	0.0146	0.0015	0.0796	0.9747	0.9747	0.016	0.0009	0.0561	0.6213
DMC+1-Heptanol																				
A_0	-18.142	-3.246	-0.219	7.642	0.104	-21.192	-3.483	-0.252	6.823	0.125	-23.784	-3.533	-0.278	5.994	0.138	-26.858	-3.953	-0.309	5.811	0.146
A_1	15.04	1.003	0.187	-5.504	-0.145	12.771	0.795	0.156	-5.133	-0.12	6.153	0.613	0.075	-5.162	-0.059	7.462	0.579	0.088	-5.374	-0.065
A_2	19.492	-0.115	0.244	-5.496	-0.179	10.073	-0.679	0.128	-2.599	-0.091	2.645	-5.151	0.037	-1.256	0.002	1.654	-2.322	0.025	-6.424	-0.01

A_3	-20.497	-0.272	-0.256	6.505	0.202	-14.92	0.156	-0.184	6.494	0.138	-0.725	0.740	-0.012	6.941	0.007	-0.526	1.57	-0.01	8.135	0.000
A_4	-16.084	-0.011	-0.205	6.951	0.157	-6.717	-1.235	-0.088	0.298	0.076	0.118	6.289	-0.0004	-3.536	-0.038	-4.418	-0.112	-0.05	2.968	0.037
σ	0.1320	0.0121	0.0017	0.0600	0.0013	0.1262	0.0097	0.0015	0.0472	0.0011	0.1506	0.0467	0.0018	0.0464	0.0015	0.0936	0.0199	0.0011	0.0473	0.0008
DMC+1-Octanol																				
A_0	-15.812	-2.767	-0.192	166.055	0.072	-18.994	-3.005	-0.227	5.947	0.094	-22.203	-3.288	-0.262	5.556	0.116	-24.934	-3.532	-0.288	5.19	0.126
A_1	20.757	1.555	0.257	-40.454	-0.191	16.376	1.629	0.200	-7.343	-0.145	9.936	0.078	0.119	-7.146	-0.076	9.549	0.646	0.111	-8.351	-0.070
A_2	18.891	-1.006	0.239	-34.012	-0.171	8.964	-0.131	0.117	-1.872	-0.085	-0.268	-6.735	0.004	-3.852	0.035	-1.802	-4.226	-0.014	-7.194	0.030
A_3	-31.652	-0.202	-0.396	-10.977	0.309	-18.361	-1.332	-0.229	9.598	0.183	-2.068	3.287	-0.03	9.800	0.007	2.831	2.659	0.028	13.675	-0.028
A_4	-17.938	2.817	-0.234	65.291	0.161	-3.712	-0.142	0.057	1.105	0.045	7.578	11.454	0.085	3.055	-0.128	7.528	5.319	0.086	8.948	-0.086
σ	0.2178	0.0165	0.0027	0.9747	0.0021	0.1253	0.0202	0.0015	0.0858	0.0012	0.1359	0.0744	0.0016	0.0843	0.0015	0.1618	0.0358	0.0019	0.1365	0.0014

Excess Molar Volume

Figure 1(a), 2(a) and 3(a) shows that for all three systems, the values of VE are negative at the temperatures under study and across the molefraction range for the three systems respectively. In its pure state, alkanols have a lot of hydrogen bonds, and the DMC has dipole-dipole interactions. When these two are mixed, the hydrogen bonds that already exist in the alkanols dissociate, forming new, strong hydrogen bonds between the carbonyl oxygen atom of DMC molecules and the hydrogen atom of the hydroxyl group of alkanols. Additionally, the structural contributions from the favorable of small DMC molecules accommodate interstitially into the voids existed in larger alkanol molecules result in a more compressed solution assembly in these mixtures.

Others have similarly reached a similar conclusion for binary mixes that comprise compounds with significant molar volume differences[18,19]. The order of V^E magnitude is decreased from 1-hexanol to 1-octanol. The interstitial accommodation and intermolecular hydrogen bonding may be a cause for negative sign in V^E.

The excess molar volumes at various temperatures exhibit parabolic curves, and it is evident that at the same temperature, they decrease as the alcohols' carbon chains lengthen. The poorer self - association in higher alcohols may be the cause of the drop in V^E with alcohol carbon chain length.

As the steric hindrance increases with the alkanols' chain length from C6 to C8, the interaction between DMC and alkanol molecule decreases, hence, the interactions' strength should follow the order: 1-hexanol >1 - heptanol >1- octanol. Thus, the negative deviation level supports our interpretation. Comparable behaviour in V^E with composition has also been stated[20] in some binary mixtures.

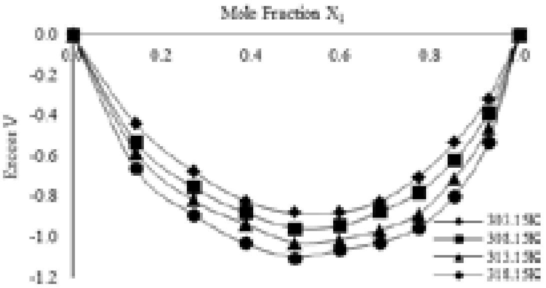

Fig. 1(a). Variation of Deviation in Excess Molar Volume with the mole fraction of DMC For DMC+1-Hexanol

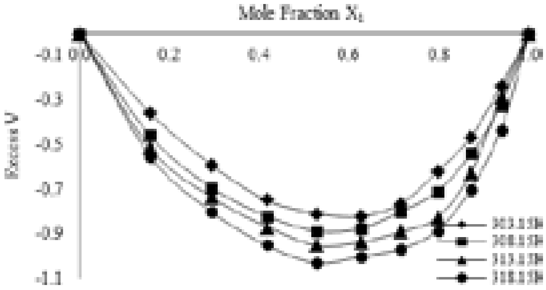

Fig. 2(a). Variation of Deviation in Excess Molar Volume with the mole fraction of DMC For DMC+Heptanol

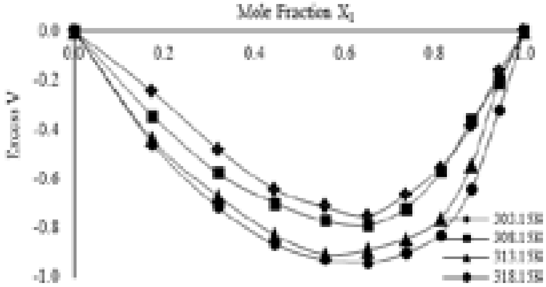

Fig. 3(a). Variation of Deviation in Excess Molar Volume with the mole fraction of DMC For DMC+1-Octanol

Intermolecular Free Length (L_f^E)

Another crucial acoustic metric for examining the type and degree of intermolecular interactions is the negative L_f^E. Sound waves must travel a relatively shorter distance between molecules in these combinations, as indicated by the negative L_f^E values for these mixtures (Fig. 1(b), 2(b) and 3(b)). This suggests that there are stronger connections and associations in these mixtures than in the perfect mixture or those pure components. Intermolecular hydrogen bonds and the favorable interstitial accommodation of dissimilar molecules in these mixes may be responsible for the more compact packing.

The degree of negative L_f^E for these combinations follows the order 1-hexanol > 1-> 1-heptanol> 1-octanol due to the more favorable interstitial accommodation of smaller DMC molecules into vacancies in alkanols, which leads in a lessening in intermolecular freelength. The L_f^E values decrease as the temperature increases, possibly as a result of the large alkanol molecules more easily accommodating the small DMC molecules in the interstitial region. As a result, the trends of L_f^E with altering DMC molefraction and the behavior of V^E are strongly in agreement.

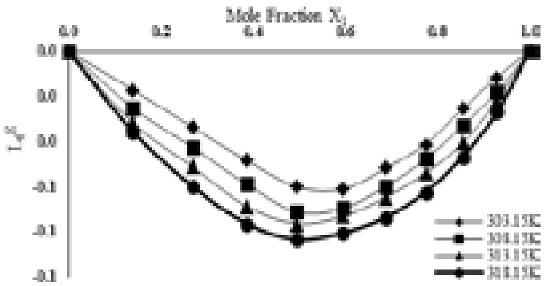

Fig. 1(b). Variation of Deviation in Excess Inter Molecular Free Length with the mole fraction of DMC For DMC+1-Hexanol

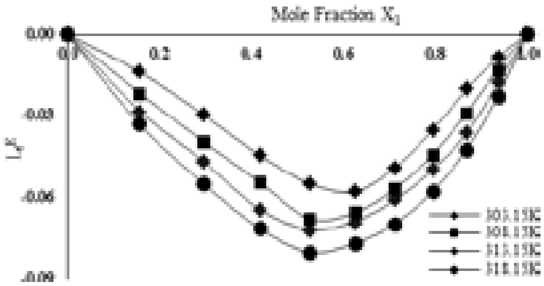

Fig. 2(b). Variation of Deviation in Excess Inter Molecular Free Length with the mole fraction of DMC For DMC+Heptanol

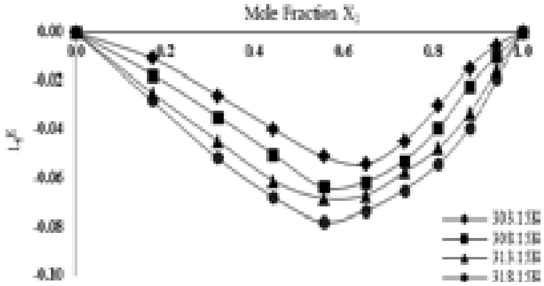

Fig. 3(b). Variation of Deviation in Excess Inter Molecular Free Length with the mole fraction of DMC For DMC+Octanol

Deviation in Adiabatic Compressibility ($\Delta\beta_{ad}$)

Adiabatic compressibility studies in binary liquid mixtures involving hydrogen bonding were conducted[21]. They claimed that the negative contribution to βad was caused by strong interactions through hydrogen bonds between dissimilar molecules.

The system's total compressibility will undoubtedly be more affected by the closer molecular packing brought about by the development of strong interaction between hetero molecules. By taking into account the following elements, the divergence in adiabatic compressibility can be explained: (1) a decrease in velocity and an increase in compressibility due to the loss of dipolar connection and the size and shape differences between the constituent molecules.

Hydrogen-bonded complexes formation

or dipole-dipole interactions between dissimilar molecules causes a decrease in compressibility and an increase in sound velocity. The resulting effect determines the actual divergence. The hydrogen bound production predominates over the other contribution, as indicated by the negative excess compressibility in each of the three systems.

Figure 1(c), 2(c) and 3(c) illustrates how $\Delta\beta_{ad}$ varies for each of the four binary systems at the various study temperatures. Over the whole composition range, the compressibility deviates negatively, reaching broad maximum at roughly 0.40 mole fractions of DMC in all the studied systems. According to these studies, hetero-molecular interactions are stronger and mixes have a tendency to pack closer together, which results in a lower compressibility phase in the intermediate composition range. Measurements of viscosity support this finding even further.

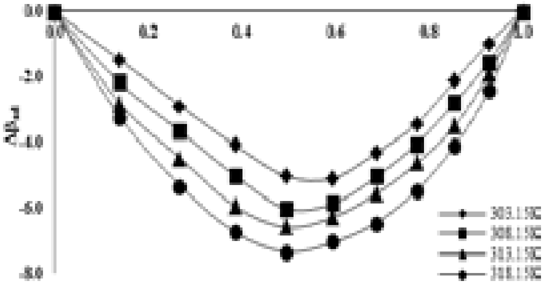

Fig. 1(c). Variation of Deviation in Adiabatic Compressibility with the mole fraction of DMC for DMC + 1-Hexanol

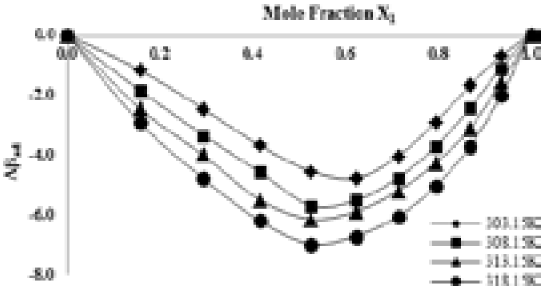

Fig. 2(c). Variation of Deviation in Adiabatic Compressibility with the mole fraction of DMC for DMC + Heptanol

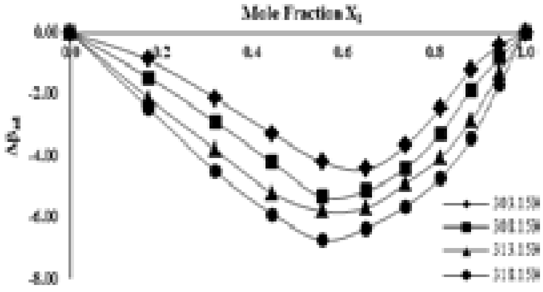

Fig. 3(c). Variation of Deviation in Adiabatic Compressibility with the mole fraction of DMC for DMC + Octanol

Excess Acoustic Impedance (Z^E)

The measure of the impedance provided by the liquid to acoustic waves propagating through it is called the acoustic impedance, and it is correlated with both the inertial and elastic properties of the medium[22]. For all of the binary systems at temperatures under study, Fig. 1(d), 2(d) and 3(d) shows positive ZE values throughout the mole fraction range. Negative/ positive ZE deviations indicate weak/strong unification between the constituent molecules in the mixtures[23,24].

The hydrogen bonds establishment between DMC and alkanol molecules is due to the geometric accommodation of small DMC molecules into the voids created by the large alkanols molecules result in a more compact solution structure, as indicated by the observed positive ZE values. This makes it challenging for sound waves to travel through the solution. 1-hexanol >1-heptanol >1-octanol is the sequence in which the magnitude of ZE values follow, suggesting the of interactions' magnitude in the similar order.

Deviation in Viscosity ($\Delta\eta$)

Fort and Moore[21] claim that as contact strength rises, viscosity deviation tends to be more positive. Viscosity variation can be used to qualitatively measure the intensity of intermolecular interactions[25]. Pikkarainan[26] claims that the following factors can be taken into consideration in order to explain the variance in viscosities. Specific interactions between dissimilar components, such as the formation of hydrogen bonds and charge-transfer complexes, may result in an increase in viscosity in mixtures as compared to the pure components. (i) Variations in the size and shape of component molecules, as well as the absence of dipolar linkage in pure components, may result in a decrease in viscosity. According to the author, the latter impact results in a positive departure in viscosity, while the former effect creates a negative divergence.

Table 3 demonstrates that the values of $\Delta\eta$ for the binary systems are positive across the entire solvent composition range at the temperatures under investigation. Positive values of Δη are observed at the temperatures under investigation indicate certain forces are acting in the mixtures. Δη values are negative in studies where dipolar and dispersion interactions are present, but dipole-dipole interactions between similar molecules and other forces produced positive values.

Table 3 demonstrates that for DMC+ hexanol systems, the values of Δη are positive over the whole solvent composition ranges at the temperatures under investigation. According to Sharma *et al.,*[27,28], the positive excess viscosities, Δη, are typically seen in systems with particular interactions of hydrogen bond formation, high dipole-dipole forces, etc. between component molecules.

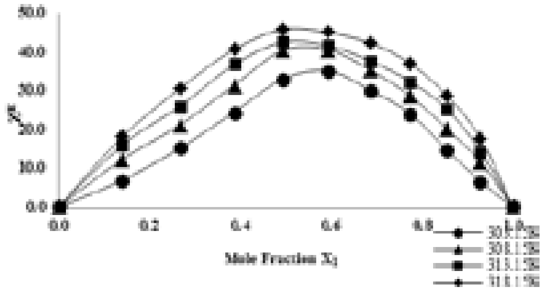

Fig. 1(d). Variation of Deviation in Excess Acoustic Impedance with the mole fraction of DMC For DMC+1-Hexanol

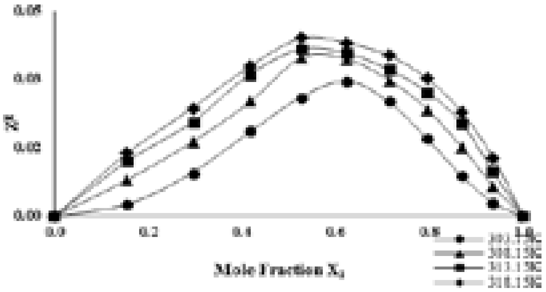

Fig. 2(d). Variation of Deviation in Excess Acoustic Impedance with the mole fraction of DMC For DMC+1-Heptanol

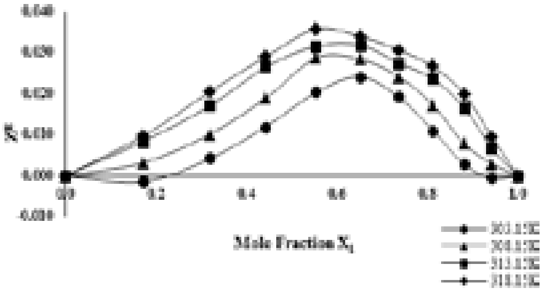

Fig. 3(d). Variation of Deviation in Excess Acoustic Impedance with the mole fraction of DMC For DMC+1-Octanol

Conversely, dispersion forces are indicated by negative Δη values[29]. The current study's binary mixtures' positive Δη values can be explained by dipole-dipole interactions that lead to the creation of hydrogen bonds and electron-transfer complexes between dissimilar molecules. Fig. 1(e), 2(e) and 3(e) display the plots of Δη against x1, and Table 3 displays the values.

Examining this figure closely reveals that the plots are parabolic and have distinct minima at a mole fraction of 0.5, which suggests that complex formation between the mixing components is present. The combined impact of variables such as molecular size, shape, and intermolecular forces determines the sign and magnitude of the viscosity deviation.

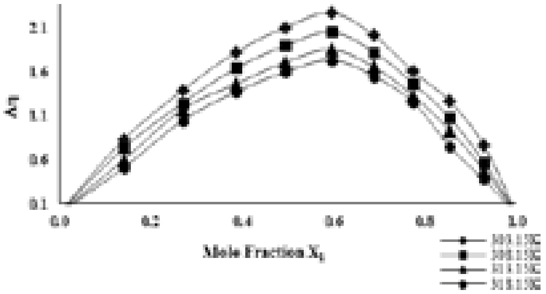

Fig. 1(e). Variation of Deviation in Excess Viscosity with the mole fraction of DMC For DMC+1-Hexanol

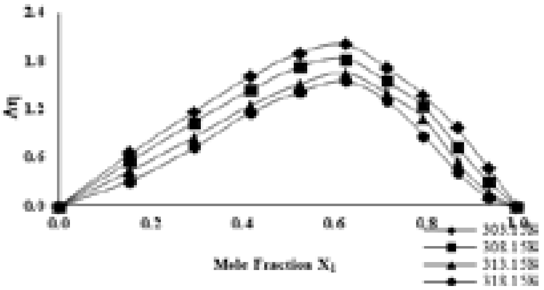

Fig. 2(e). Variation of Deviation in Excess Viscosity with the mole fraction of DMC For DMC+Heptanol

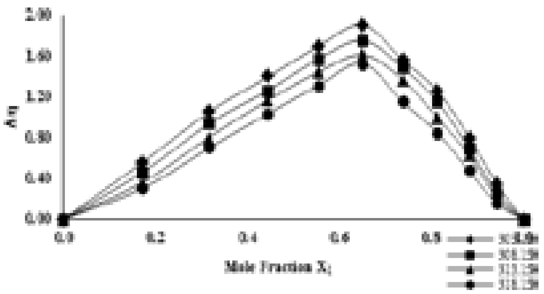

Fig. 3(e). Variation of Deviation in Excess Viscosity with the mole fraction of DMC For DMC+Octanol

In their study, Sankar reported a specific interaction that results in positive deviations in viscosities. Gowrisankar[29] found binary combinations of N-Methyl Aniline with some ketones, as well as amine and cyclic ketones mixtures. Certain forces that strengthened the intermolecular contacts between the solvent molecules were responsible for the binary mixes' positive contribution of $\Delta\eta$.

CONCLUSION

Density, ρ, and sound speed experimental data are shown, for DMC+1-hexanol,+1-heptanol, and 1-octanol mixes over the whole molefraction range at all studies temperatures T = (303.15 - 318.15)K. Over the whole composition range, excess metrics such as V^E, $\Delta\beta_{ad}$, L_f^E, $\Delta\eta$ and Z^E were assessed. The results showed that there were intermolecular interactions between DMC and alkanol molecules because of their strong hydrogen bonding and as the molecular size difference between them, which allowed smaller DMC molecules to fit interstitial into the voids left by larger alkanol molecules. The DMC-alkanol interactions in these combinations are in the following sequence, according to the magnitudes of the excess properties: 1-hexanol >1- heptanol >1-octanol.

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Conflict of interest

The author declare that we have no conflict of interest.

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