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Ultrasonic Studies in the Binary Mixtures of Dimethyl Carbonate with Some Aliphatic Esters

G. Jyothirmai[1,4], P. B. Sandhya Sri[2], Ch. Anajaneyulu[3]
[1]*Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar, Guntur-522510, Andhra Pradesh, India*
[2]*Department of Physics & Electronics, KBN College, Vijayawada-520001, Andhra Pradesh, India*
[3]*Department of Physics, Bapatla Engineering College, Bapatla 522101, AP, India*
[4] *Department of Physics, Govt. Degree College, Avanigadda-52121, Andhra Pradesh, India*

Abstract
The binary mixes Di Methyl Carbonate (DMC) + Methyl Acetate (MA), + Ethyl Acetate (EA), and + Butyl Acetate (BA) were measured for ultrasonic velocity (U), density (ρ), and viscosity (η) at four different temperatures (303.15-318.15K) covering the whole composition range. Deviations in adiabatic compressibility and viscosity, as well as excess values of molar volume, intermolecular free length, and relaxation time, were computed from the experimental data. To find binary constants and the standard deviation (σ) between the estimated and experimental values, the Redlich-Kister polynomial equation has been fitted to the values of V^E, $\Delta\beta_{ad}$, L_f^E, $\Delta\eta$.

Keywords: Di methyl carbonate, Densities, Speed of sound, Viscosity Compressibilities, Molar volumes, Inter Molecular Free Lengths.

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I. Introduction

In the majority of engineering computations, where fluid flow or mixing plays a significant role in numerous real-world issues pertaining to mass transport applications, the physical characteristics of liquid mixes are necessary. DMC has a dipole moment of 0.90 D and is a polar, aprotic solvent. DMC is primarily utilized as an intermediate in the synthesis of different polymers and in the electrolytes of lithium-ion batteries, which are anticipated to be crucial for energy storage, as well as in the manufacturing of biodiesel and building materials like paints and cleaning and degreasing agents. On the other side, esters are used as plasticizers in the polymer processing industry to promote thermoplastic behaviour [1-3]. It is crucial to comprehend how DMC mixes with esters because this knowledge may be useful in a variety of engineering fields. At 303.15, 308.15, and 313.15 K, we present the density, viscosity, and sound speed findings for the binary mixes of DMC with methyl acetate, ethyl acetate, n-butyl acetate, and n-butyl acetate across the whole composition range. This information has been used to calculate the excess molar volume, viscosity deviations, sound speed deviations, adiabatic compressibility deviation, acoustic impedance, and excess Gibbs free energy of activation of viscous flow. To determine the binary coefficients and standard deviation, these findings were fitted to the Redlich-Kister polynomial equation using a multiparametric nonlinear regression analysis technique.

II. Experimental Techniques

a) Measurement of Velocity

The formula U=λf can be used to calculate the ultrasonic velocity. The frequency of the generator employed in the investigation is 2 MHz. To get the high frequency generator's anode current meter to read its maximum, a micrometer screw and a lot of work were required. While adjusting the micrometer screw for n peaks, we should note how many times the anode current was at its highest.

$$d = n\lambda/2$$

Multiplying the displacement of the reflector by 20 peaks by 100 makes it easy to determine the speed in meters per second. Since the distance 'd' can be determined with a micrometer to an accuracy of 0.01 mm or more, the quality of the distance measurement largely determines the velocity's precision.

b) Measurements of Density

In the current investigation, a specific gravity bottle with a 5ml volume was used to test the density (ρ) for pure liquids and all liquid combinations at various temperatures between 303.15K and 318.15K with a 5K interval. One of the factors utilized to assess the liquids' purity was their density. To achieve thermal equilibrium, the specific gravity bottle was placed in the thermostat for fifteen minutes. When they reach room temperature, they are taken out of the thermostat and weighed. There is a 0.5 mg margin of error in the density readings.

c) Measurements of Viscosity

At 303.15, 308.15, 313.15, and 318.15K, the viscosity was measured using a 0.55mm diameter Ubbelohde capillary viscometer that was calibrated using double-distilled water. The viscometer is calibrated using pure water, and the liquid is allowed to stand in a thermostatic water bath for about half an hour to minimize temperature swings. The precision of the viscosity measurements is 0.005 mPas.

III. Theoretical Considerations

i) Molar volume

$$V = M/\rho \qquad 3.1$$

ii). Excess Volume (V^E)

$$V^E = V - (V_1X_1+V_2X_2) \qquad 3.2$$

where X_1 indicates the mole fractions of common compound and X_2 indicates the molefraction of sub compound and V_1 & V_2 are the mean molar volumes respectively.

iii). Adiabatic Compressibility (β_{ad})

$$\beta_{ad} = 1/\rho U^2 \qquad 3.3$$

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

$$\Delta\beta_{ad} = \beta_{ad} - (\beta_{ad1}X_1 + \beta_{ad2}X_2) \qquad 3.4$$

where pure liquids' adiabatic compressibilities are indicated as β_{ad1} and $\beta_{ad2.}$

v). Intermolecular free length (L_f)

$$L_f = K(\beta_{ad})^{1/2} \qquad 3.5$$

Jacobson constant is indicated as K.

vi). Excess Intermolecular free length (L_f^E)

$$L_f^E = L_f - (L_{f1}X_1 + L_{f2}X_2) \qquad 3.6$$

pure liquids' intermolecular free length are L_{f1} and L_{f2} respevtively

vii). Deviation in Viscosity ($\Delta\eta$)

The equation for deviation in viscosity is

$$\Delta\eta = \eta_{mix} - (X_1\eta_1+X_2\eta_2) \qquad 3.7$$

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

The excess/deviation values of $\Delta\beta_{ad,}$ V^E, $\Delta\eta$, L_f^E, were least squares fitted to the Redlich – Kister type polynomial[4]

$$Y^E = X(1-X)\sum_{i=1}^{n} A_i(1-2X)^{i-1} \qquad 3.8$$

The coefficients of A_i in the above equation along with the standard deviation (Y^E) are given in Tables. These coefficients are the adjustable parameters to get best - fit values of Y^E which are indicated in the table along with standard deviations (Y^E) calculated by using the following relation

$$\sigma Y^E = \sum \left[\frac{\left[Y^E_{exp} - Y^E_{cal} \right]^2}{m - n} \right]^{1/2} \quad 3.9$$

Theoretical Velocities

Nomoto[5] developed the following ratio for liquid mixes assuming the additivity of molar sound velocity (R) and no volume change upon mixing

$$U_N = \left[\frac{X_1 R_1 + X_2 R_2}{X_1 V_1 + X_2 V_2} \right]^3 \quad 3.10$$

According to Blandamer and Waddington's [6] assumptions, the ideal mixing theory put forth by Van Dael and Vangeel [7] yields the following relation for ultrasonic velocity in liquid mixtures:

$$\frac{1}{\left[X_1 M_1 + X_2 M_2 \right] \left[U_{imx} \right]^2} = \frac{X_1}{M_1 U_1^2} + \frac{X_2}{M_2 U_2^2} \quad 3.11$$

where U_{imx} is the liquid mixture's optimal ultrasonic mixing velocity.Ultrasonic velocity in species is represented by U_1 and U_2.

Impedance Relation

Using the specific acoustic impedance of the pure liquids, the ultrasonic speed in the liquid mixtures is determined using the following relation[8]

$$U_{Imp} = \frac{\sum X_i Z_i}{\sum X_i \rho_i} \quad 3.12$$

Where X_i s the molefraction, Z_i acoustic impedance and ρ_i is the density

Using the ratio of the temperature coefficient of speed and expansion coefficient, Rao[9] derived a formula for ultrasonic speed (U_R) given by

$$U_R = \left[\frac{R}{V} \right]^3 \quad 3.13$$

where V is the molar volume and R is called Rao's constant or molar sound speed,which is constant for a liquid at a temperature.Junjie [10] assumed that the ultrasonic speed of the mixture depends on the mole fraction, molecular weight and density of the mixture. Junjie's relation is given by

$$U_J = \frac{\left[\frac{X_1 M_1}{\rho_1} + \frac{X_2 M_2}{\rho_2} \right]}{\left[X_1 M_1 + X_2 M_2 \right]^{1/2} \left[\frac{X_1 M_1}{\rho_1 U_1^2} + \frac{X_1 M_1}{\rho_1 U_1^2} \right]^{1/2}} \quad 3.14$$

ix Chi-square test for goodness of fit

As indicated by Karl Pearson [11], Chi-square value is evaluated for the binary liquid mixtures under study utilizing the formula

$$\chi^2 = \frac{\left[U_{obs} - U_{Cal} \right]^2}{U_{Cal}} \quad 3.15$$

where n is the number of data used, and U (obs) = experimental values of ultrasonic velocities U(cal) = computed values of ultrasonic velocities

x Relative Percentage Error

The Average percentage error is calculated by utilizing the relation

$$APE = \frac{1}{n}\sum\left[\frac{U_{obs} - U_{cal}}{U_{obs}}\right]\times 100 \qquad 3.16$$

xi Molecular Association

The degree of intermolecular interaction or molecular association is given by

$$\alpha = \frac{U_{exp}^2}{U_{imx}^2} - 1 \qquad 3.17$$

IV. Solvent purification

Because the purity of the liquid affects the accuracy and precision of the results, it is imperative to utilize the purest components available. When creating several purification methods, which are detailed in the literature, the type and functional groups of the compounds were taken into account [12,13].

Table-1: Literature Data in comparison with experimental data at 303.15K

Liquid	Density(ρ) Kg/m³		Velocity of Ultrasonic Sound(U)m/s		Viscosity(η) cP	
	Exptl	Lit	Exptl	Lit	Exptl	Lit
DMC	1.0562	1.05671[14]	1175.3	1177[14]	0.549	0.549[14]
MA	0.9206	0.9201[15]	1106	1106.5[15]	0.372	0.3514[15]
EA	0.8885	0.8884[15]	1117.3	1122.8[15]	0.382	0.3995[15]
BA	0.8716	0.8712[15]	1165.2	1176.4[15]	0.643	0.6407[15]

V. Results & Discussion

Tables 2, summarize excess characteristics of DMC with methyl, ethyl, and n-butyl acetate calculated by using the values of density, ultrasonic velocity, viscosity, andat temperatures ranging from 303.15 to 318.15K. Table 3 shows the values of parameters A_0, A_1, A_2, A_3, and A_4 derived by least squares analysis, along with their standard deviation.

Figs 1(a), 1(b) and 1(c) illustrate the relationship between excess volume (V^E) and DMC mole fraction at various temperatures. The main causes of volume expansion, or positive V^E values, are

(i) Chemical interactions between constituent molecules, such as the creation of H-bonds.

(ii) Association through weaker physical forces, such as dipolar force or other similar factors.

(iii) Molecules from one component are accommodated in the interstitial places of the other's structural network.

The strength of unlike molecular interactions in a solution can be assessed by the sign and magnitude of V^E. V^E values are negative across all three systems. However, methyl acetate has significantly higher negative V^E values compared to other esters. The lower size of methyl acetate molecules in the DMC dipole network suggests interstitial accommodation. The negative V^E values at higher temperatures suggest the interstitial accommodation of methyl acetate molecules [16].

DMC with aliphatic esters have algebraic V^E values about 303.15K followed the order:

MA>EA>BA

Volume expansion is caused by the breaking up of molecular clumps or dipolar molecules, as well as dispersion forces between molecules.

The sign of a system's V^E is determined by the relative expansion and contraction of the two liquids during mixing. Previous studies reported similar results [17].

The development of hydrogen bonds and dipole-dipole interactions between hetero molecules can significantly impact the system's compressibility. The differences in adiabatic compressibility can be explained by the following reasons.

a) Differences in size and shape of component molecules reduce velocity and increase compressibility.

b) Dipole-dipole interaction or hydrogen bonding between molecules leads to increased sound velocity and decreased compressibility.

The actual deviation is determined by the resulting effect. Figures 1(b), 2(b) and 2(c) show negative deviations in adiabatic compressibilities over DMC mole fractions, showing significant interactions between molecules.

$\Delta\beta_{ad}$ values are consistently negative across all compositions and intensify at increasing temperatures. The structure of homologous series of esters has a significant impact on adiabatic compressibility. Figures 1(b), 2(b) and 2(c) show that when the ester chain length decreases, the $\Delta\beta_{ad}$ values become increasingly negative.

In this investigation, the behavior of V^E and $\Delta\beta_{ad}$ are comparable. The sign of $\Delta\beta_{ad}$ supports the postulates used to understand the excess molar volume sign. Negative V^E and $\Delta\beta_{ad}$ values may be caused by dipole-dipole and dipole-induced dipole interactions. [15-18] that improve the solvent structure of the mixture, hence lowering V^E and $\Delta\beta_{ad}$.

Table 2: Excess/deviation values of calculated thermodynamic parameters for DMC + MA, EA and BA systems at 303.15, 308.15, 313.15 and 318.15K

DMC+Methyl Acetate					DMC+Ethyl Acetate					DMC+Butyl Acetate				
X_1	$_{ad}$	V^E	(L_f^E)	( )	X_1	$_{ad}$	V^E	(L_f^E)	( )	X_1	$_{ad}$	V^E	(L_f^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
0.0949	-4.5347	-0.2162	-0.0477	0.3050	0.1144	-3.8711	-0.1754	-0.0399	0.2620	0.1479	-4.6004	-0.1473	-0.0499	0.4780
0.1909	-7.6496	-0.4521	-0.0821	0.5910	0.2252	-6.5265	-0.4004	-0.0687	0.5390	0.2809	-7.4888	-0.3654	-0.0832	0.9440
0.2879	-9.7808	-0.6340	-0.1070	0.7700	0.3326	-8.6687	-0.5895	-0.0935	0.7030	0.4011	-9.5824	-0.5533	-0.1089	1.1930
0.3861	-11.2247	-0.7699	-0.1250	0.9180	0.4367	-9.9526	-0.7270	-0.1095	0.8340	0.5102	-11.0311	-0.6929	-0.1278	1.3240
0.4855	-12.2569	-0.8458	-0.1390	0.9940	0.5376	-10.8296	-0.8105	-0.1216	0.8890	0.6098	-11.5313	-0.7818	-0.1356	1.3220
0.5860	-11.5478	-0.7412	-0.1324	0.8860	0.6356	-10.5332	-0.6898	-0.1201	0.8520	0.7010	-11.3980	-0.6689	-0.1356	1.1840
0.6876	-9.4760	-0.6137	-0.1091	0.7690	0.7307	-8.5880	-0.5637	-0.0985	0.7220	0.7848	-9.6627	-0.5207	-0.1154	0.9940
0.7905	-7.0899	-0.4755	-0.0821	0.5400	0.8230	-6.4461	-0.4218	-0.0744	0.4820	0.8621	-7.4704	-0.3789	-0.0894	0.6790
0.8946	-4.3851	-0.2587	-0.0511	0.2710	0.9128	-3.2247	-0.2009	-0.0372	0.2260	0.9336	-3.9486	-0.1668	-0.0470	0.4030
1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	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
0.0949	-5.0185	-0.2685	-0.0528	0.2420	0.1144	-4.9962	-0.2689	-0.0508	0.2190	0.1479	-5.6198	-0.2277	-0.0604	0.3140
0.1909	-7.9970	-0.5295	-0.0856	0.4730	0.2252	-8.0229	-0.4865	-0.0833	0.4760	0.2809	-9.4916	-0.4900	-0.1048	0.7500
0.2879	-10.3259	-0.6901	-0.1126	0.6500	0.3326	-9.8396	-0.6830	-0.1042	0.6270	0.4011	-11.5439	-0.7005	-0.1301	0.9820
0.3861	-11.5639	-0.8131	-0.1280	0.8270	0.4367	-11.3715	-0.8457	-0.1230	0.7260	0.5102	-13.3871	-0.8485	-0.1539	1.1220
0.4855	-12.6706	-0.8914	-0.1426	0.8950	0.5376	-12.6148	-0.9123	-0.1396	0.7810	0.6098	-13.6246	-0.9118	-0.1586	1.1420
0.5860	-12.0016	-0.7929	-0.1364	0.8060	0.6356	-12.2780	-0.7926	-0.1379	0.7420	0.7010	-13.7541	-0.8146	-0.1622	1.0060
0.6876	-9.8703	-0.6804	-0.1126	0.6520	0.7307	-10.4970	-0.6792	-0.1189	0.6160	0.7848	-12.2357	-0.6508	-0.1450	0.8490
0.7905	-7.7038	-0.5213	-0.0884	0.4240	0.8230	-8.1593	-0.5325	-0.0931	0.4340	0.8621	-9.1008	-0.4859	-0.1076	0.5520
0.8946	-4.8068	-0.3226	-0.0554	0.2160	0.9128	-4.7174	-0.2616	-0.0540	0.1770	0.9336	-5.2100	-0.2290	-0.0613	0.2840
1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	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
0.0949	-5.7767	-0.2966	-0.0598	0.1770	0.1144	-6.0802	-0.3397	-0.0612	0.1850	0.1479	-6.5898	-0.3076	-0.0698	0.2400
0.1909	-9.0076	-0.5597	-0.0949	0.3630	0.2252	-9.2734	-0.5952	-0.0953	0.4070	0.2809	-11.1844	-0.5982	-0.1219	0.6140
0.2879	-11.2967	-0.7271	-0.1211	0.5310	0.3326	-11.2594	-0.7910	-0.1180	0.5630	0.4011	-13.9161	-0.8483	-0.1551	0.8340
0.3861	-12.6280	-0.8390	-0.1374	0.7100	0.4367	-13.1673	-0.9566	-0.1411	0.6480	0.5102	-15.8768	-0.9949	-0.1805	0.9730
0.4855	-13.4475	-0.9199	-0.1486	0.7860	0.5376	-14.2926	-1.0434	-0.1564	0.6860	0.6098	-16.1829	-1.0459	-0.1864	1.0000
0.5860	-12.9357	-0.8409	-0.1445	0.7120	0.6356	-14.2522	-0.9493	-0.1586	0.6630	0.7010	-16.1554	-0.9469	-0.1883	0.8650
0.6876	-10.9417	-0.7297	-0.1228	0.5810	0.7307	-12.5272	-0.8064	-0.1407	0.5410	0.7848	-14.6675	-0.8100	-0.1719	0.7460
0.7905	-8.6832	-0.5714	-0.0981	0.3660	0.8230	-10.0490	-0.6361	-0.1138	0.3810	0.8621	-10.9704	-0.5961	-0.1280	0.4740
0.8946	-6.1202	-0.3626	-0.0697	0.1570	0.9128	-5.6227	-0.3225	-0.0636	0.1430	0.9336	-6.0565	-0.3347	-0.0700	0.2180
1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	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
0.0949	-6.1921	-0.3423	-0.0626	0.1290	0.1144	-7.3333	-0.4316	-0.0720	0.1690	0.1479	-7.4716	-0.3653	-0.0777	0.1790
0.1909	-9.8957	-0.6038	-0.1020	0.2980	0.2252	-10.6427	-0.7074	-0.1065	0.3580	0.2809	-12.6020	-0.6777	-0.1350	0.5190
0.2879	-12.2489	-0.7710	-0.1284	0.4620	0.3326	-12.7974	-0.9021	-0.1306	0.5080	0.4011	-15.6177	-0.9711	-0.1711	0.7300
0.3861	-13.6647	-0.8821	-0.1455	0.6220	0.4367	-14.6496	-1.0718	-0.1529	0.5850	0.5102	-17.6717	-1.1186	-0.1975	0.8610
0.4855	-14.5588	-0.9476	-0.1574	0.7190	0.5376	-15.7172	-1.1710	-0.1676	0.6250	0.6098	-18.1998	-1.1471	-0.2063	0.9150
0.5860	-13.9105	-0.8757	-0.1520	0.6550	0.6356	-15.4819	-1.0861	-0.1678	0.6070	0.7010	-18.0051	-1.0673	-0.2063	0.7830
0.6876	-11.8995	-0.7705	-0.1308	0.5120	0.7307	-14.0245	-0.9510	-0.1539	0.4900	0.7848	-16.3085	-0.9465	-0.1877	0.6580
0.7905	-9.5702	-0.6156	-0.1059	0.3030	0.8230	-11.2197	-0.7350	-0.1241	0.3490	0.8621	-12.2912	-0.6905	-0.1408	0.3990
0.8946	-6.7261	-0.3949	-0.0750	0.1150	0.9128	-6.8441	-0.4104	-0.0759	0.1250	0.9336	-7.0927	-0.3900	-0.0805	0.1710
1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000

Figures 3(a), 3(b) and 3(c) show how excess free length varies across DMC compositions in the three systems studied. According to Ramamurthy and Sastry [19], negative L_f^E values suggest that sound waves must travel a greater distance. This could be due to dominating interactions between different molecules. The presence of ad and L_f^E minima at the same concentrations supports molecular connections.

Fig 4(a), 4(b) and 4(c) show negative viscosity deviations for all binary systems across the mole fraction range, with negative maximum values around 0.4 mole fractions. Viscosity varies based on the strength

of interactions between like and unlike molecules. The sign and magnitude of Δη vary with the structural features of liquid components due to differences in molecular size and shape, resulting from geometrical fitting.

Negative variations in viscosity may be caused by dispersion or dipolar forces between molecules due to their size and shape differences.

Physical interactions are often weak or strong, and the sign of Δη might be negative or positive. Positive values of Δη indicate strong intermolecular interactions, while negative values indicate lesser interactions between dissimilar molecules.

Specific chemical interactions between liquid mixture components, such as hydrogen bond formation and dipole-dipole interactions, cause the structure to become more compact and result in positive viscosity deviations. The sign and magnitude of Δη vary with the structural features of liquid components, resulting from geometrical fitting due to differences in molecular size and shape. In this scenario, all three systems have negative Δη values, indicating strong interactions such as interstitial accommodation. The results are in good agreement with those derived from data based on V^E and deviations in compressibility ($\Delta\beta_{ad}$)

Table 4 & 5 shows the actual values as well as the theoretical values computed using the Nomoto, Van Dael ideal mixing, impedance, Rao's specific velocity, and Junjie relationships for the analyzed systems at temperatures of 303.15, 308.15, 313.15, and 318.15K along with percentage of deviations. The validity of various theoretical formulae is evaluated by percentage deviation and chi square test for all the mixtures at all the temperatures, which are also shown in Table 4 & 5. It is assumed that all molecules are spherical, although this is not always the case. Nomoto's hypothesis assumes that the volume remains constant when mixed. As a result, no interactions between liquid mixture components were considered. The assumption for the establishment of an ideal mixing relation is that the specific heat ratios of ideal mixtures and volumes are equal. Again, no molecular interactions are taken into consideration.

Table 3: Experimental and theoretical velocities of DMC + MA, EA and BA systems using various theories

DMC+Methyl Acetate							
X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	U_{KUD}
303.15K							
0.0000	1106.0	1106.0	1106.0	1106.0	1106.0	1106.0	1106.0
0.0949	1138.7	1111.8	1113.4	1111.9	1110.0	1128.7	1114.1
0.1909	1165.2	1117.8	1120.8	1118.0	1114.4	1151.0	1121.8
0.2879	1187.6	1124.1	1128.0	1124.3	1119.4	1169.8	1129.3
0.3861	1207.0	1130.6	1135.1	1130.9	1124.9	1185.1	1136.6
0.4855	1225.2	1137.3	1142.0	1137.6	1131.1	1196.4	1143.5
0.5860	1230.0	1144.3	1148.9	1144.6	1138.0	1198.1	1150.3
0.6876	1222.6	1151.6	1155.7	1151.9	1145.8	1197.3	1156.9
0.7905	1212.8	1159.2	1162.3	1159.4	1154.5	1194.4	1163.2
0.8946	1201.0	1167.1	1168.9	1167.2	1164.3	1186.5	1169.3
1.0000	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3
308.15K							
0.0000	1102.9	1102.9	1102.9	1102.9	1102.9	1102.9	1102.9
0.0949	1136.5	1107.2	1108.4	1107.3	1105.6	1126.2	1108.8
0.1909	1160.0	1111.6	1113.7	1111.9	1108.7	1148.0	1114.4
0.2879	1182.0	1116.2	1119.0	1116.6	1112.2	1164.2	1119.9
0.3861	1197.6	1120.9	1124.2	1121.4	1116.2	1177.2	1125.2
0.4855	1214.0	1125.9	1129.3	1126.4	1120.7	1186.7	1130.3
0.5860	1217.0	1131.0	1134.4	1131.5	1125.8	1186.8	1135.3
0.6876	1207.3	1136.3	1139.3	1136.8	1131.6	1184.6	1140.1
0.7905	1198.0	1141.9	1144.2	1142.2	1138.1	1178.8	1144.8
0.8946	1183.0	1147.7	1149.0	1147.9	1145.4	1169.6	1149.3
1.0000	1153.7	1153.7	1153.7	1153.7	1153.7	1153.7	1153.7
313.15K							
0.0000	1083.5	1083.5	1083.5	1083.5	1083.5	1083.5	1083.5
0.0949	1120.1	1087.8	1089.0	1088.0	1086.3	1107.5	1089.4
0.1909	1144.5	1092.3	1094.5	1092.6	1089.5	1129.0	1095.2
0.2879	1165.6	1097.0	1099.8	1097.3	1093.1	1145.2	1100.7
0.3861	1181.8	1101.8	1105.1	1102.2	1097.2	1157.6	1106.1
0.4855	1195.5	1106.8	1110.3	1107.3	1101.8	1167.1	1111.3
0.5860	1200.1	1112.0	1115.4	1112.5	1106.9	1168.3	1116.3
0.6876	1192.6	1117.4	1120.4	1117.8	1112.8	1166.4	1121.2

0.7905	1183.5	1123.0	1125.3	1123.4	1119.3	1160.9	1126.0
0.8946	1172.6	1128.9	1130.2	1129.1	1126.7	1151.8	1130.5
1.0000	1135.0	1135.0	1135.0	1135.0	1135.0	1135.0	1135.0
318.15K							
0.0000	1062.9	1062.9	1062.9	1062.9	1062.9	1062.9	1062.9
0.0949	1099.2	1067.1	1068.3	1067.3	1065.6	1088.3	1068.7
0.1909	1125.3	1071.5	1073.6	1071.7	1068.6	1109.3	1074.3
0.2879	1145.9	1076.0	1078.8	1076.4	1072.1	1125.2	1079.7
0.3861	1162.0	1080.7	1083.9	1081.1	1076.0	1137.4	1084.9
0.4855	1176.0	1085.5	1089.0	1086.0	1080.5	1146.1	1090.0
0.5860	1179.6	1090.6	1093.9	1091.1	1085.5	1147.4	1094.9
0.6876	1172.8	1095.9	1098.8	1096.3	1091.2	1145.8	1099.6
0.7905	1164.1	1101.3	1103.6	1101.7	1097.6	1140.4	1104.2
0.8946	1152.2	1107.1	1108.4	1107.2	1104.8	1130.9	1108.7
1.0000	1113.0	1113.0	1113.0	1113.0	1113.0	1113.0	1113.0

Table 4 Percentage Deviations and Interaction Parameters (α)

DMC+Ethyl Acetate

X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	U_{KUD}
303.15K							
0.0000	1117.3	1117.3	1117.3	1117.3	1117.3	1117.3	1117.3
0.1144	1147.0	1123.0	1125.0	1123.4	1120.4	1130.2	1124.2
0.2252	1171.0	1128.7	1132.2	1129.4	1124.1	1145.0	1130.9
0.3326	1193.6	1134.5	1138.9	1135.3	1128.3	1158.6	1137.2
0.4367	1211.3	1140.3	1145.1	1141.2	1133.1	1170.3	1143.3
0.5376	1227.0	1146.1	1151.0	1147.0	1138.5	1180.0	1149.2
0.6356	1234.0	1151.9	1156.4	1152.8	1144.5	1181.5	1154.8
0.7307	1225.5	1157.7	1161.6	1158.5	1151.1	1182.4	1160.2
0.8230	1215.0	1163.5	1166.4	1164.1	1158.4	1182.3	1165.4
0.9128	1195.1	1169.4	1171.0	1169.7	1166.5	1178.6	1170.5
1.0000	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3
308.15K							
0.0000	1095.2	1095.2	1095.2	1095.2	1095.2	1095.2	1095.2
0.1144	1130.0	1101.0	1103.0	1101.3	1098.3	1111.2	1102.2
0.2252	1156.0	1106.7	1110.2	1107.3	1102.0	1125.6	1108.9
0.3326	1175.7	1112.5	1117.0	1113.3	1106.3	1139.4	1115.3
0.4367	1195.0	1118.3	1123.3	1119.2	1111.1	1152.1	1121.4
0.5376	1214.0	1124.2	1129.2	1125.1	1116.5	1161.2	1127.3
0.6356	1221.2	1130.0	1134.7	1130.9	1122.6	1163.0	1133.0
0.7307	1215.2	1135.9	1139.9	1136.7	1129.3	1164.6	1138.5
0.8230	1204.1	1141.8	1144.7	1142.4	1136.7	1164.6	1143.7
0.9128	1184.0	1147.8	1149.4	1148.1	1144.8	1159.2	1148.8
1.0000	1153.7	1153.7	1153.7	1153.7	1153.7	1153.7	1153.7
313.15K							
0.0000	1080.7	1080.7	1080.7	1080.7	1080.7	1080.7	1080.7
0.1144	1120.0	1086.0	1087.9	1086.4	1083.5	1098.4	1087.2
0.2252	1146.0	1091.4	1094.7	1092.0	1086.9	1113.6	1093.4
0.3326	1166.3	1096.8	1100.9	1097.6	1090.8	1126.9	1099.3
0.4367	1188.0	1102.2	1106.8	1103.1	1095.2	1139.3	1105.0
0.5376	1205.5	1107.6	1112.2	1108.5	1100.2	1148.8	1110.5
0.6356	1215.0	1113.0	1117.4	1113.9	1105.9	1151.2	1115.8
0.7307	1210.0	1118.5	1122.2	1119.3	1112.1	1151.5	1120.9
0.8230	1198.2	1124.0	1126.7	1124.6	1119.0	1150.3	1125.8
0.9128	1170.7	1129.5	1131.0	1129.8	1126.7	1143.1	1130.5
1.0000	1135.0	1135.0	1135.0	1135.0	1135.0	1135.0	1135.0
318.15K							
0.0000	1052.4	1052.4	1052.4	1052.4	1052.4	1052.4	1052.4
0.1144	1096.0	1058.3	1060.5	1058.7	1055.7	1073.3	1059.6
0.2252	1122.0	1064.3	1068.0	1064.9	1059.6	1089.6	1066.6
0.3326	1143.4	1070.3	1075.0	1071.1	1064.0	1103.4	1073.2
0.4367	1164.7	1076.3	1081.5	1077.2	1069.0	1116.4	1079.6
0.5376	1182.1	1082.4	1087.6	1083.3	1074.6	1127.0	1085.7
0.6356	1191.0	1088.4	1093.3	1089.3	1080.8	1130.6	1091.6
0.7307	1190.0	1094.5	1098.7	1095.3	1087.8	1132.1	1097.3
0.8230	1178.0	1100.7	1103.7	1101.3	1095.4	1130.0	1102.7
0.9128	1153.9	1106.8	1108.5	1107.2	1103.8	1123.4	1107.9
1.0000	1113.0	1113.0	1113.0	1113.0	1113.0	1113.0	1113.0

DMC+Methyl Acetate

X_1	$\%U_N$	$\%U_{imp}$	$\%U_{UVDV}$	$\%U_{UJUN}$	$\%U_{URAO}$	$\%U_{KUD}$	U^2/U^2_{imx}
X_1	UEXP	UNOM	UIMP	UVDV	UJUN	URAO	UKUD
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
303.15K							
0.0949	-2.3572	-2.2138	-2.3484	-2.5189	-0.8779	-2.1603	1.0487	0.0487
0.0000	1165.2	1165.2	1165.2	1165.2	1165.2	1165.2	1165.2
0.1909	-4.0652	-3.8135	-4.0492	-4.3592	-1.2197	-3.7231	1.0862	0.0862
0.1479	1203.0	1166.5	1167.0	1166.6	1163.9	1152.3	1166.4
0.2879	-5.3480	-5.0205	-5.3267	-5.7449	-1.5014	-4.9072	1.1157	0.1157
0.2809	1230.0	1167.7	1168.4	1167.9	1163.3	1147.5	1167.6
0.3861	-6.3329	-5.9607	-6.3082	-6.8015	-1.8110	-5.8366	1.1392	0.1392
0.4011	1251.7	1168.8	1169.7	1169.1	1163.4	1147.2	1168.7
0.4855	-7.1755	-6.7893	-7.1493	-7.6813	-2.3524	-6.6652	1.1599	0.1599
0.5102	1268.4	1169.9	1170.8	1170.2	1164.1	1150.0	1169.7
0.5860	-6.9676	-6.5940	-6.9417	-7.4773	-2.5897	-6.4784	1.1548	0.1548
0.6098	1276.0	1170.9	1171.8	1171.2	1165.2	1155.2	1170.7
0.6876	-5.8105	-5.4777	-5.7868	-6.2842	-2.0720	-5.3784	1.1266	0.1266
0.7010	1277.9	1171.9	1172.7	1172.1	1166.6	1156.7	1171.7
0.7905	-4.4206	-4.1618	-4.4018	-4.8055	-1.5191	-4.0874	1.0942	0.0942
0.7848	1262.8	1172.8	1173.4	1173.0	1168.4	1159.4	1172.7
0.8946	-2.8258	-2.6768	-2.8147	-3.0576	-1.2103	-2.6356	1.0588	0.0588
0.8621	1242.6	1173.7	1174.1	1173.8	1170.5	1164.3	1173.6
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.9336	1210.4	1174.5	1174.7	1174.6	1172.8	1168.2	1174.5
1.0000	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
308.15K							
0.0949	-2.5809	-2.4752	-2.5675	-2.7171	-0.9045	-2.4408	1.0534	0.0534
0.0000	1149.4	1149.4	1149.4	1149.4	1149.4	1149.4	1149.4
0.1909	-4.1732	-3.9874	-4.1491	-4.4209	-1.0332	-3.9290	1.0884	0.0884
0.1479	1192.0	1149.9	1150.1	1150.0	1147.5	1138.1	1149.9
0.2879	-5.5688	-5.3271	-5.5367	-5.9023	-1.5072	-5.2539	1.1207	0.1207
0.2809	1225.5	1150.5	1150.8	1150.5	1146.3	1134.0	1150.4
0.3861	-6.4016	-6.1262	-6.3641	-6.7954	-1.7029	-6.0456	1.1406	0.1406
0.4011	1246.0	1151.0	1151.3	1151.0	1145.8	1133.8	1150.9
0.4855	-7.2592	-6.9731	-7.2193	-7.6833	-2.2514	-6.8924	1.1617	0.1617
0.5102	1265.7	1151.4	1151.8	1151.5	1145.9	1136.5	1151.3
0.5860	-7.0661	-6.7891	-7.0266	-7.4925	-2.4815	-6.7137	1.1569	0.1569
0.6098	1270.5	1151.8	1152.2	1151.9	1146.4	1140.4	1151.8
0.6876	-5.8775	-5.6304	-5.8413	-6.2730	-1.8788	-5.5654	1.1279	0.1279
0.7010	1274.6	1152.3	1152.6	1152.3	1147.3	1142.1	1152.2
0.7905	-4.6834	-4.4914	-4.6546	-5.0033	-1.6067	-4.4427	1.1000	0.1000
0.7848	1261.7	1152.6	1152.9	1152.7	1148.5	1143.9	1152.6
0.8946	-2.9861	-2.8753	-2.9691	-3.1785	-1.1365	-2.8483	1.0621	0.0621
0.8621	1232.5	1153.0	1153.2	1153.1	1150.0	1147.7	1153.0
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.9336	1197.8	1153.4	1153.7	1153.4	1151.8	1149.5	1153.3
1.0000	1153.7	1153.7	1153.7	1153.7	1153.7	1153.7	1153.7
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
313.15K							
0.0949	-2.8767	-2.7698	-2.8644	-3.0119	-1.1201	-2.7330	1.0598	0.0598
0.0000	1130.1	1130.1	1130.1	1130.1	1130.1	1130.1	1130.1
0.1909	-4.5599	-4.3721	-4.5376	-4.8054	-1.3550	-4.3097	1.0973	0.0973
0.1479	1177.0	1130.7	1131.0	1130.8	1128.3	1121.2	1130.7
0.2879	-5.8866	-5.6421	-5.8569	-6.2172	-1.7485	-5.5638	1.1283	0.1283
0.2809	1215.0	1131.3	1131.7	1131.4	1127.3	1118.2	1131.2
0.3861	-6.7651	-6.4867	-6.7305	-7.1552	-2.0423	-6.4006	1.1495	0.1495
0.4011	1241.0	1131.9	1132.3	1132.0	1126.9	1119.5	1131.8
0.4855	-7.4174	-7.1276	-7.3805	-7.8383	-2.3718	-7.0411	1.1657	0.1657
0.5102	1262.0	1132.4	1132.8	1132.5	1127.0	1122.4	1132.3
0.5860	-7.3399	-7.0598	-7.3034	-7.7625	-2.6532	-6.9791	1.1638	0.1638
0.6098	1268.0	1132.9	1133.3	1133.0	1127.6	1126.1	1132.8
0.6876	-6.3039	-6.0544	-6.2706	-6.6952	-2.1980	-5.9850	1.1383	0.1383
0.7010	1271.0	1133.4	1133.7	1133.4	1128.5	1128.0	1133.3
0.7905	-5.1100	-4.9161	-5.0835	-5.4264	-1.9098	-4.8641	1.1100	0.1100
0.7848	1258.9	1133.8	1134.1	1133.9	1129.8	1131.0	1133.7
0.8946	-3.7275	-3.6161	-3.7119	-3.9171	-1.7760	-3.5872	1.0786	0.0786
0.8621	1225.4	1134.2	1134.4	1134.3	1131.3	1133.1	1134.2
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.9336	1183.0	1134.6	1134.7	1134.6	1133.1	1134.9	1134.6
1.0000	1135.0	1135.0	1135.0	1135.0	1135.0	1135.0	1135.0
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
318.15K							
0.0949	-2.9213	-2.8130	-2.9079	-3.0596	-0.8961	-2.7779	1.0608	0.0608
0.0000	1110.4	1110.4	1110.4	1110.4	1110.4	1110.4	1110.4
0.1909	-4.7872	-4.5972	-4.7629	-5.0379	-1.4231	-4.5279	1.1025	0.1025
0.1479	1160.0	1110.7	1110.9	1110.7	1108.4	1102.8	1110.7
0.2879	-6.0078	-5.8505	-6.0655	-6.4357	-1.7993	-5.7760	1.1333	0.1333
0.2809	1200.0	1111.0	1111.2	1111.1	1107.1	1100.1	1111.0
0.3861	-6.9887	-6.7173	-6.9611	-7.3974	-2.4188	-6.6354	1.1552	0.1552
0.4011	1227.0	1111.3	1111.6	1111.4	1106.5	1102.4	1111.3
0.4855	-7.6917	-7.3989	-7.6516	-8.1220	-2.5460	-7.3168	1.1726	0.1726
0.5102	1248.0	1111.6	1111.9	1111.6	1106.4	1105.2	1111.6
0.5860	-7.5468	-7.2634	-7.5071	-7.9794	-2.7292	-7.1868	1.1689	0.1689
0.6098	1256.0	1111.9	1112.1	1111.9	1106.7	1108.1	1111.8
0.6876	-6.5621	-6.3098	-6.5259	-6.9626	-2.3067	-6.2440	1.1445	0.1445
0.7010	1257.2	1112.1	1112.3	1112.2	1107.5	1110.5	1112.1
0.7905	-5.3943	-5.1983	-5.3655	-5.7184	-2.0356	-5.1490	1.1166	0.1166
0.7848	1243.4	1112.4	1112.5	1112.4	1108.5	1114.0	1112.3
0.8946	-3.9174	-3.8046	-3.9004	-4.1119	-1.8505	-3.7773	1.0828	0.0828
0.8621	1208.7	1112.6	1112.7	1112.6	1109.8	1114.6	1112.6
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.9336	1166.0	1112.8	1112.9	1112.8	1111.3	1115.0	1112.8
1.0000	1113.0	1113.0	1113.0	1113.0	1113.0	1113.0	1113.0

DMC+Butyl Acetate

303.15K

308.15K

313.15K

318.15K

Table 5: Valus of chi-square and the standard deviation σ for the binary mixtures of DMC with MA, EA and BA at different temperatures.

	UNOM	Uimp	UVDV	UJUN	URAO	UKUD
	DMC + Methyl Acetate					
	303.15K					
	-0.4798	-0.4508	-0.4779	-0.5184	-0.1544	3.8066

x^2	30.5319	27.1595	30.2960	35.2974	3.4083	1.5939
	308.15K					
	-0.4941	-0.4725	-0.4911	-0.5265	-0.1476	4.0120
x^2	31.6775	29.1238	31.3137	35.6975	3.0856	1.7706
	313.15K					
	-0.5317	-0.5097	-0.5289	-0.5640	-0.1753	4.3149
x^2	35.2559	32.5501	34.9043	39.4212	4.0950	2.0480
	318.15K					
	0.0485	-0.0107	-0.2491	-0.0569	0.0280	4.4910
x^2	0.3653	0.01784	9.14227	0.49645	0.12337	2.21861
	DMC + Ethyl Acetate					
	303.15K					
	-0.4399	-0.4101	-0.4342	-0.4864	-0.2650	-3.6349
x^2	26.4088	23.1860	25.7746	31.8435	9.8829	1.4534
	308.15K					
	-0.5127	-0.4816	-0.5068	-0.5609	-0.3074	-4.2260
x^2	34.1142	30.3620	33.3857	40.3372	12.7680	1.9645
	313.15K					
	-0.5869	-0.5572	-0.5809	-0.6342	-0.3478	-4.8311
x^2	43.4543	39.4909	42.6406	50.1755	16.0666	2.5674
	318.15K					
	0.0485	-0.0107	-0.2491	-0.0569	0.0280	-5.1234
x^2	0.3653	0.0178	9.1423	0.4964	0.1234	2.8874
	DMC + Butyl Acetate					
	303.15K					
	-0.5859	-0.5804	-0.5842	-0.6214	-0.7117	-4.9773
x^2	46.1345	45.3527	45.8949	51.4164	65.2205	2.7251
	308.15K					
	-0.6949	-0.6925	-0.6944	-0.7292	-0.7896	-5.8268
x^2	62.6754	62.2863	62.5892	68.4422	78.4277	3.7347
	313.15K					
	-0.7998	-0.7971	-0.7992	-0.8343	-0.8589	-6.6262
x^2	80.9863	80.4855	80.8651	87.3650	91.5667	4.8298
	318.15K					
	0.0485	-0.0107	-0.2491	-0.0569	0.0280	-7.1010
x^2	0.3653	0.0178	9.1423	0.4964	0.1234	5.5467

The assumption for the establishment of an ideal mixing relation is that the specific heat ratios of ideal mixtures and volumes are equal. Again, no molecular interactions are taken into consideration. Similarly, the CFT assumes that the molecules are genuine, non-elastic entities, which is not the case. However, when two liquids are mixed, their molecules interact due to the presence of numerous types of forces such as dispersion forces, charge transfer, hydrogen bonding, dipole-dipole, and dipole-induced dipole interactions. Thus, the observed departure of predicted velocity values from practical values indicates that a molecular interaction is occurring between dissimilar molecules in the liquid mixture.

VI. Conclusion

Density, ρ, and sound speed experimental data are shown, for DMC+MA, +EA, and EA 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 VE, Δβad, LfE and Δη were assessed. The results showed that there were intermolecular interactions between DMC and acetate molecules because of their strong hydrogen bonding The DMC - acetate interactions in these combinations are in the following sequence, according to the magnitudes of the excess properties: MA > EA >BA.

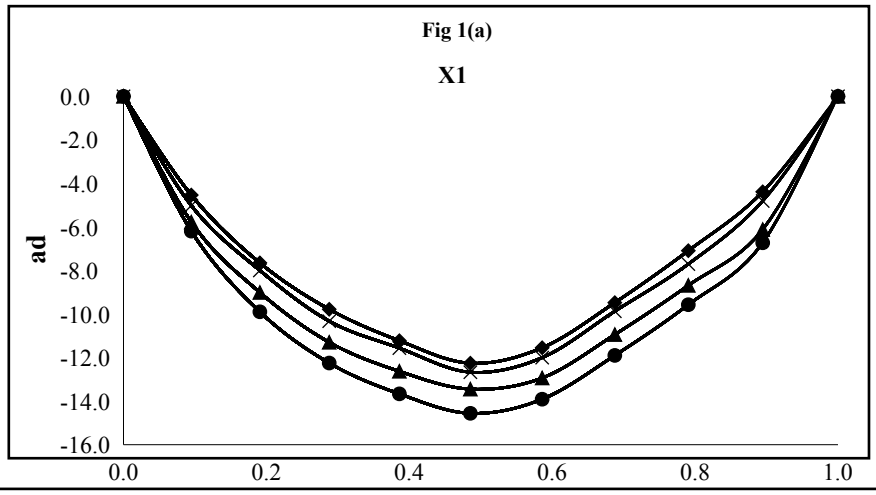


Fig 1(a)
X1
ad
0.0
-2.0
-4.0
-6.0
-8.0
-10.0
-12.0
-14.0
-16.0
0.0
0.2
0.4
0.6
0.8
1.0

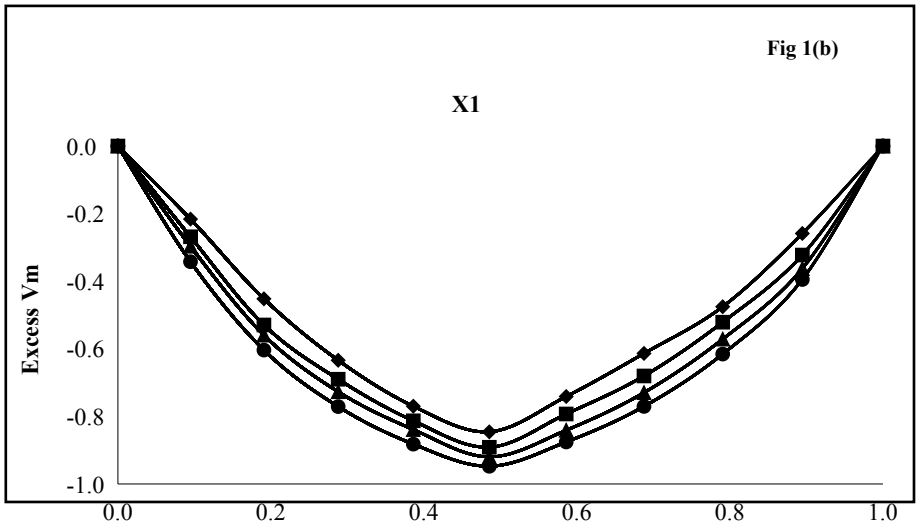


Fig 1(b)
X1
Excess Vm
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
0.0
0.2
0.4
0.6
0.8
1.0

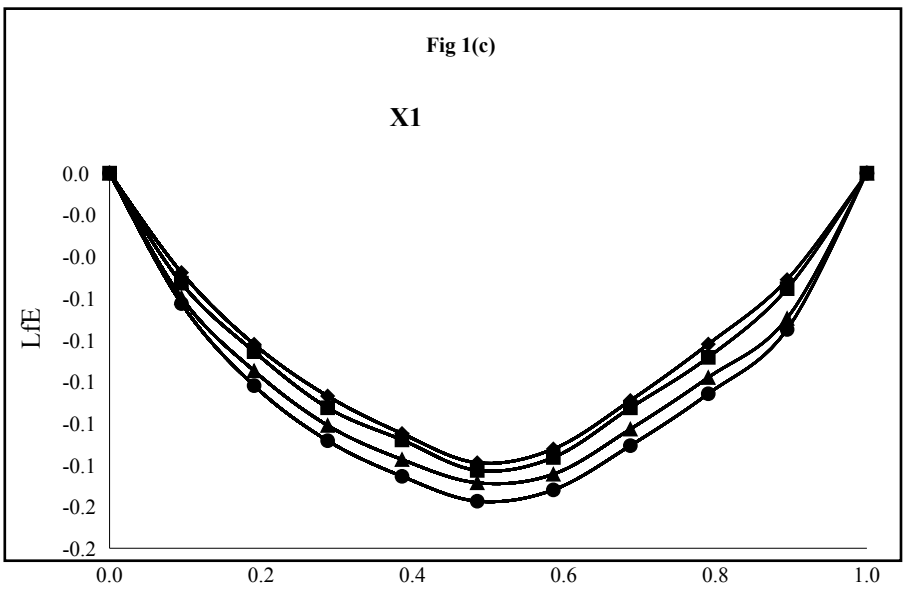


Fig 1(c)
X1
LfE
0.0
-0.0
-0.0
-0.1
-0.1
-0.1
-0.1
-0.1
-0.2
-0.2
0.0
0.2
0.4
0.6
0.8
1.0

Fig 1(d)

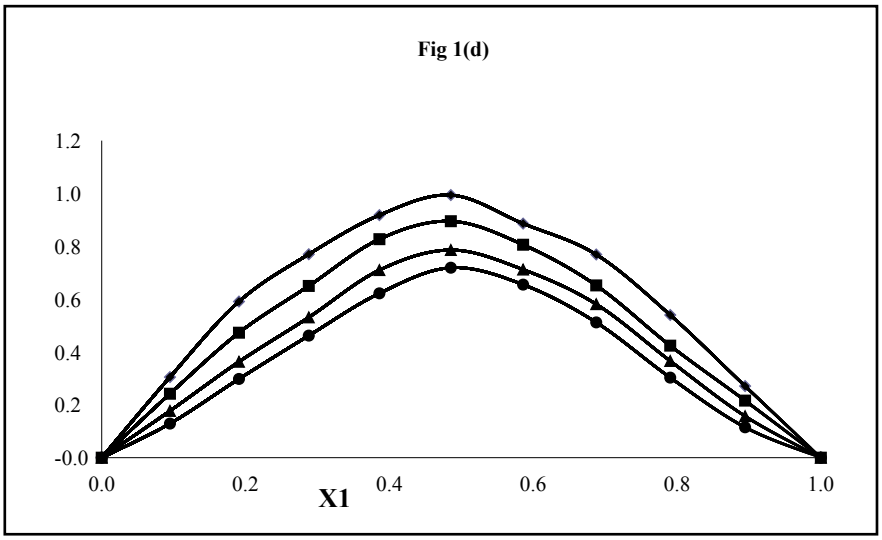


Fig 2(a)

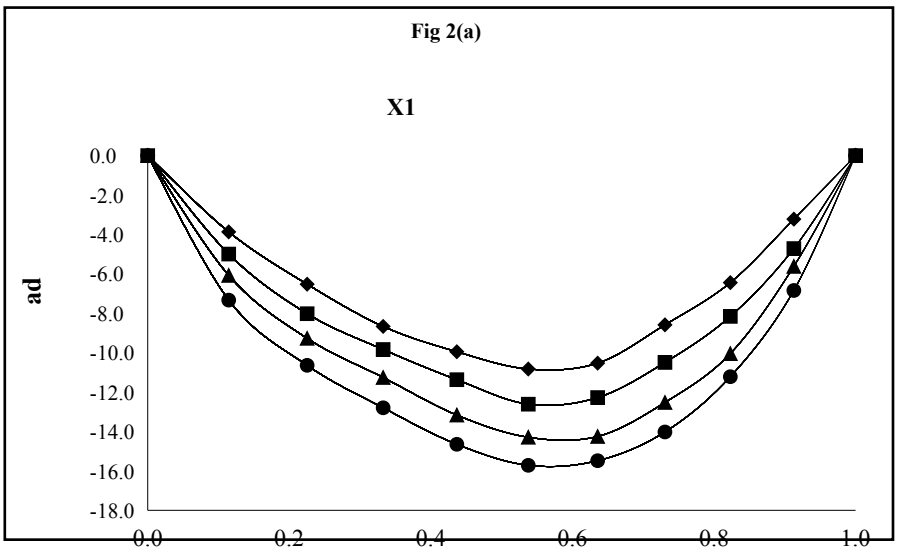


Fig 2(b)

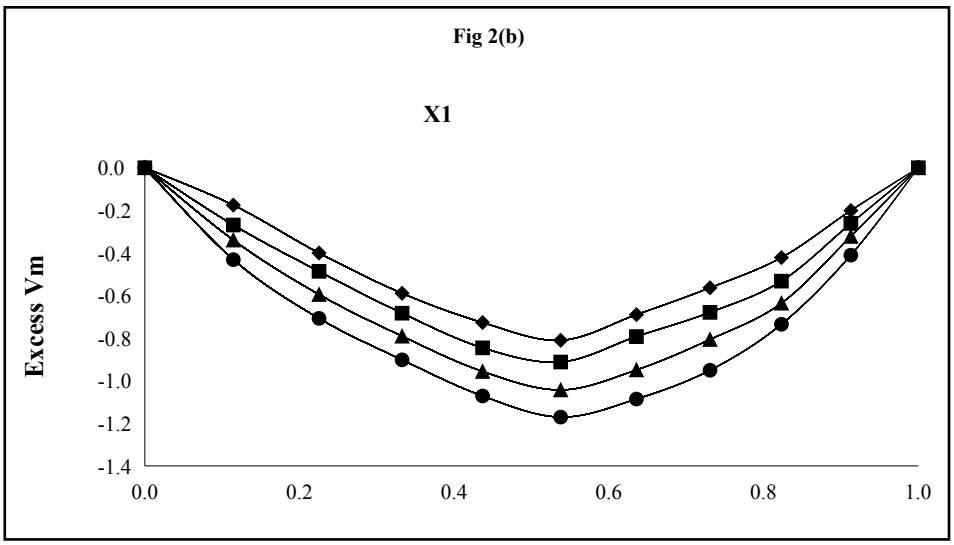


Fig 2(c)

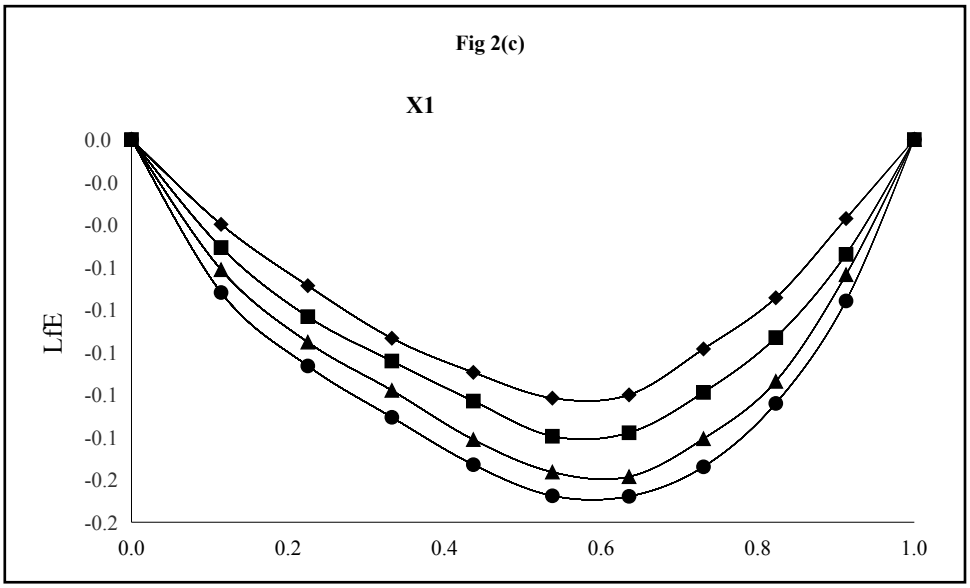


Fig 2(d)

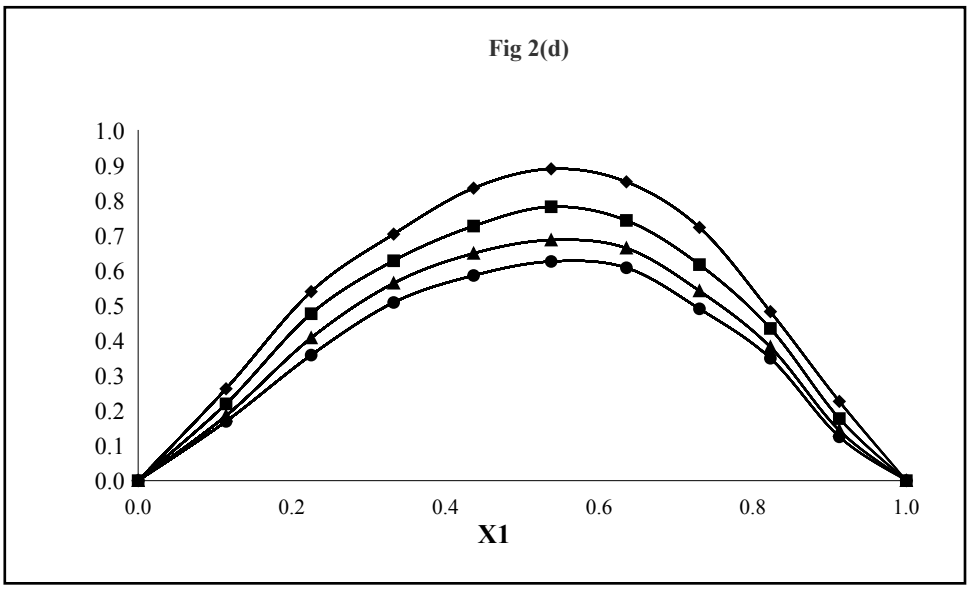
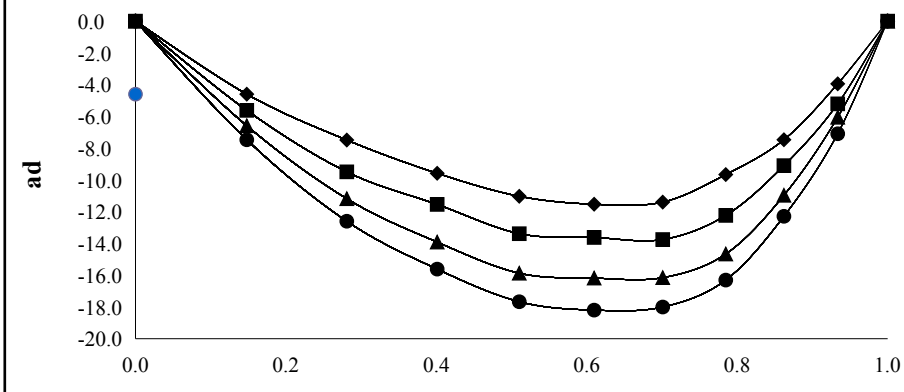
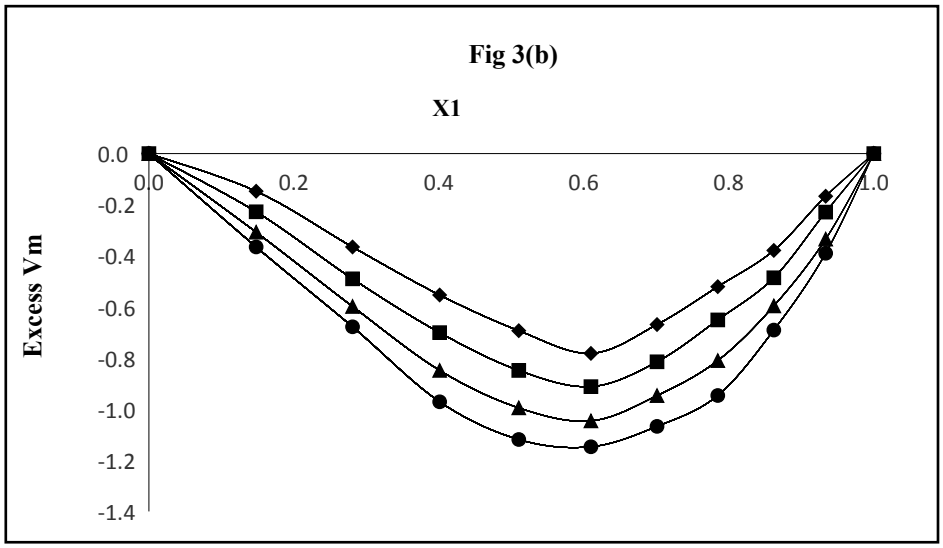
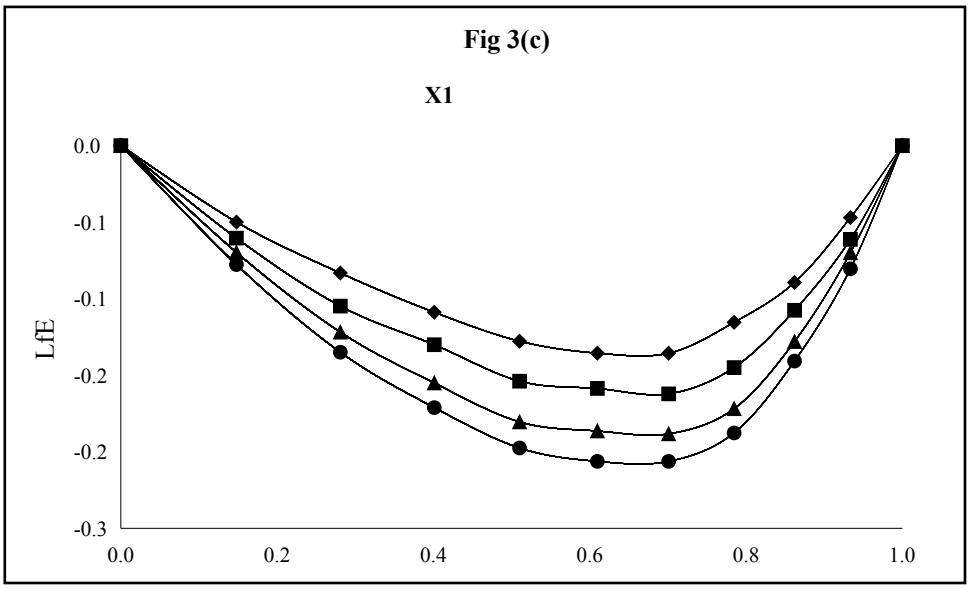


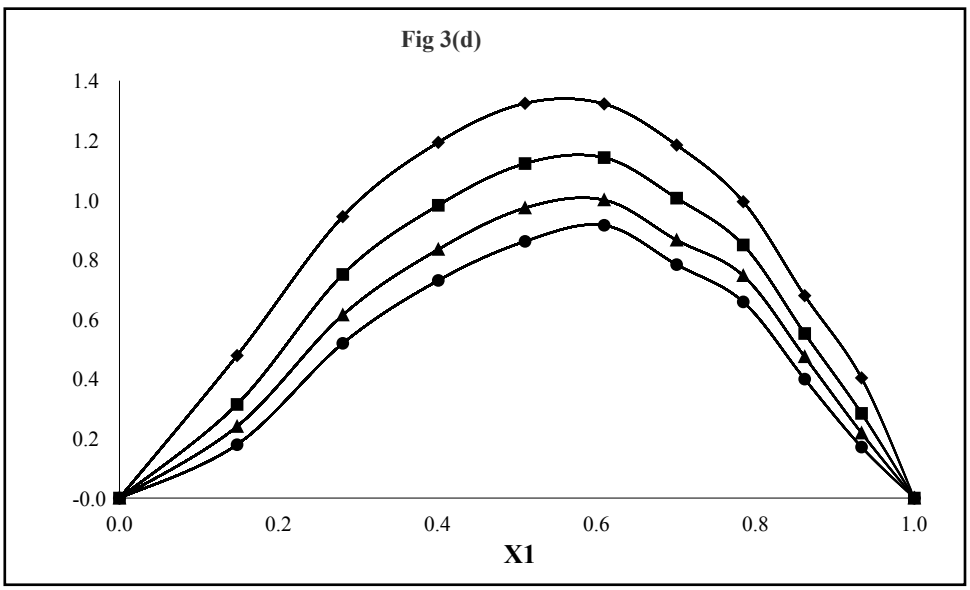
Fig 3(a)

X1









*** Followed the same for indication different temperatures in all graphs

303.15K 308.15K 313.15K 318.15K

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