Thermoacoustical studies on the binary mixtures of methyl and ethyl acetate (MA & EA) in 2-methoxyethanol (2ME) at different temperatures

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Abstract : *Density and ultrasonic velocity have been measured in the binary liquid mixtures of methyl acetate (MA) and ethyl acetate (EA) in 2-methoxyethanol (2ME) over the temperature range from 303.15 to 323.15 K. The measured data are used to compute the excess thermodynamic parameters namely excess adiabatic compressibility (β_s^E), excess intermolecular free length (L_f^E) and excess molar volume (V^E). A plot of these excess thermodynamic parameters against the mole fraction of methyl acetate and ethyl acetate over the entire composition range shows a negative deviation indicating a strong interaction between the component molecules of liquid mixtures. The results are discussed in terms of formation of hydrogen bonding between the component molecules of the liquid mixtures.*

Keywords: *ultrasonic velocity, excess adiabatic compressibility, excess free length, excess molar volume, hydrogen bonding.*

I. Introduction

The nature and the relative strength of the molecular interaction between the component molecules of liquid mixtures have been successfully investigated by many authors using ultrasonic method [1-9]. This is mainly due to the fact that the ultrasonic velocity measured in pure liquids or liquid mixtures is fundamentally related to the binding forces between atoms or molecules of a given liquid and between the component molecules in the case of liquid mixtures. The excess thermodynamic parameters calculated in liquid mixtures at various temperatures can also provide information on the nature and degree of interaction between the component molecules of the liquid mixtures. The deviation of excess thermodynamic parameters with composition from its ideal behaviour gives a deep insight into the various other dynamic processes that occur in the solutions [10-19]. In the present paper, we report on the results of nature of molecular interactions between the molecules of the binary mixtures of methylacetate (MA) and ethylacetate (EA) in 2-methoxyethanol (2ME) using excess thermodynamic parameters like excess adiabatic compressibility (β_s^E), excess intermolecular free length (L_f^E) and excess molar volume (V^E) respectively in the temperature range 303.15 - 323.15 K.

II. Materials And Method

The chemicals used in the present work are spectroscopic (SR) grade with a minimum assay of 99.9 %. These chemicals were purchased from SD Fine chemicals, India. The purity of the chemicals is checked by recording the IR spectrum of each of these chemicals and comparing it with the standard spectrum available in the literature. In all systems studied, the various compositions of the binary liquid mixtures were prepared in terms of mole fraction. The density and ultrasonic velocity were measured as a function of composition of the binary mixtures at 303.15, 308.15, 313.15, 318.15 and 323.15 K respectively. The density of pure liquids and their liquid mixtures are measured using a dilatometer of 20 ml capacity with the dilatometer immersed in a temperature controlled water bath (accuracy ±0.01°C). The accuracy in the measurement of density of pure liquids and their liquid mixtures is ±2 parts in 10^4. The ultrasonic velocity of the liquid mixtures has been measured using a Digital Ultrasonic Velocity meter (Model VCT-70A, Vi-Microsystems Pvt. Ltd., Chennai, India) in the temperature range of 303.15 - 323.15 K by circulating water from a thermostatically controlled water bath and the temperature being maintained to an accuracy of ±0.01°C. Using the measured values of ultrasonic velocity and density, various excess thermodynamic parameters such as excess adiabatic compressibility (βs^E), excess free length (L_f^E) and excess molar volume (V^E) have been calculated using the equations,

$$\beta_s^{\,E} = \beta_{s12} - \beta_{cal} \qquad\qquad (1)$$

where

$$\left(\beta_s\right)_{cal} = X_1\beta s_1 + X_2\beta s_2$$

$$L_f^E = L_{f12} - \left(L_f\right)_{cal} \tag{2}$$

where

$$\left(L_f\right)_{cal} = X_1 L_{f1} + X_2 L_{f2}$$

$$V^E = V_{obs} - V_{cal} \tag{3}$$

where $\quad V_{obs} = \left[\dfrac{X_1 M_1 + X_2 M_2}{\rho_{12}}\right]$

$$V_{cal} = \left[\dfrac{X_1 M_1}{\rho_1} + \dfrac{X_2 M_2}{\rho_2}\right]$$

where M_1, M_2, X_1, X_2, ρ_1, ρ_2, ρ_{12}, βs_1, βs_2, βs_{12}, L_{f1}, L_{f2}, L_{f12} are the molecular weight, mole fraction, density, adiabatic compressibility and intermolecular free length of the components 1 and 2 and their mixtures respectively. All the excess thermodynamic parameters were fitted to Redlich-Kister equation

$$Y^E = X_1 X_2 \sum_{j=1}^{N} A_{j-1} (2X_1 - 1)^{j-1} \tag{4}$$

and the parameters A_{j-1} were computed using least square fit method.

III. Results And Discussion

The ultrasonic velocity measurements are carried out in the binary mixtures of methyl acetate-2methoxyethanol (MA-2ME) and ethyl acetate-2methoxyethanol (EA-2ME) at different temperatures. The experiment was carried out in the composition range of X_1=0 to 1 mole fraction of methyl and ethyl acetates. The measured density and the density values reported in the literature for methyl acetate, ethyl acetate and 2-Methoxyethanol are given in Table1. Using the measured values of ultrasonic velocity and density for the binary mixtures of MA-2ME and EA-2ME are calculated and are presented in Tables 2 & 3. The coefficients of equation (4) viz., A_0 to A_3 computed for βs^E, L_f^E and V^E by least square fitting method along with the standard deviations (σ) are given in Tables 4 & 5. The variation of excess thermodynamic parameters such as excess adiabatic compressibility (βs^E), excess freelength (L_f^E) and excess molar volume(V^E) with increasing concentration of methyl and ethyl acetates (X_1 = 0 to 1 mole fraction) are shown in figures 1-6.

3.1 METHYL ACETATE – 2 METHOXYETHANOL SYSTEM (MA-2ME)

Figure 1 shows that the excess adiabatic compressibility at 303.15 K has a negative deviation for the entire concentration range of methyl acetate. The magnitude of negative deviation reaches a maximum at X_1=0.4983 mole fraction of MA and then becoming less and less negative with further increase in concentration of MA in 2ME. The excess free length and excess molar volume also exhibits a similar behaviour as that of excess adiabatic compressibility at 303.15 K. The observed negative deviation of βs^E, L_f^E and V^E at 303.15 K from the ideal behaviour can be explained as follows;

Generally, liquid mixtures which show non-linearity in ultrasonic velocity with concentration can be analysed in terms of excess thermodynamic functions. This is due to the fact that the excess thermodynamic functions are found to be sensitive towards the mutual interactions between the component molecules of the liquid mixture. In ideal mixtures, the physical property of the mixture may be evaluated as a sum of fractional contribution from the individual components. But, non-ideal mixtures show considerable deviation from linearity in their physical property with respect to concentration and these have been interpreted as arising due to strong or weak interactions. The sign and the extent of deviation of these functions from ideality depend on the nature of constituents and composition of the mixtures [20,21].

The negative deviation exhibited by excess adiabatic compressibility at 303.15 K becomes increasingly negative reaching a maximum at X_1= 0.4983 mole fraction of MA. This may be due to increasing strength of interaction between the components of liquid mixture. The greater negative deviation of βs^E for MA-2ME system suggests that a specific molecular interaction is likely to operate between 2ME and MA molecules leading to the formation of a complex. In MA-2ME system, 2ME is a highly associated liquid and MA is highly polar and also a proton acceptor. Hence, in the present binary mixture MA-2ME, in general the interaction responsible for association may be likely due to hydrogen bonding, dipole-dipole interactions or formation of complexes due to charge transfer. In MA-2ME system, the complex formation may be through hydrogen

bonding between 2ME and MA molecules. From the structure of the molecules of the constituents, it can be inferred that the oxygen atom of carbonyl group (C=O) of MA may be involved in O-H---O bonding with the hydroxyl group (OH) of 2ME molecule with the strength of bonding becoming maximum at X_1= 0.4983 mole fraction of MA . The present study is supported by the ultrasonic studies carried in the binary mixtures of dimethylsulphoxide - acetone carried out by Syal et al [22], and in some monohydric alcohols in dimethylsulphoxide carried out by Palani et al [23].

L_f^E at 303.15 K also shows negative deviation for the entire composition range of MA showing maximum negative deviation at X_1 =0.4983 mole fraction of MA (Figure.2). The negative deviation in L_f^E indicates that ultrasonic waves cover a longer distance due to decrease in intermolecular free length describing the dominant nature of hydrogen bonding between unlike molecules of the binary mixture. A similar type of studies was reported by Rajagopal and Chenthilnath [15] in the binary mixtures of 2- methyl-2 propanol in acetophenone.

The excess molar volume (V^E) for MA-2ME system in the temperature range studied also shows a negative deviation for the entire composition range of MA with the maximum negative deviation occurring at X_1= 0.4983 mole fraction (Figure 3). The changes in V^E is influenced by two factors namely,
(i) loss of dipolar association and differences in size and shape and
(ii) dipole-dipole, dipole-induced dipole interaction, charge transfer complexation and hydrogen bonding between unlike molecules.

The former effect leads to expansion in volume and the latter contributes a contraction in volume. The actual value of V^E depends on the balance between these two opposing contributions [24]. Large negative values of V^E indicate strong interaction between unlike molecules [11]. Such a large negative deviation in V^E is observed in the present MA-2ME system. The greater negative deviation is due to the formation of hydrogen bonding between 2ME and MA molecules.

As the temperature is increased to 308.15, 313.15, 318.15 and 323.15 K, the maximum negative deviation of βs^E, L_f^E and V^E further increases and is more pronounced at 323.15 K compared to their values in other temperatures respectively. This indicates that the complex formation is more favoured at 323.15 K rather than at other temperatures. This can be explained as follows:

At 303.15 K, 2ME is self associated through hydrogen bonding. At higher temperatures due to thermal agitation, self associated 2ME molecules are disrupted, and this facilitates the interaction between 2ME and MA molecules through the formation of intermolecular hydrogen bonding. Thus, at a higher temperature of 323.15 K, probably the interaction is stronger than that at other temperatures. This observation is further supported by the conclusions drawn by Chauhan et al. [25], in their ultrasonic velocity studies carried out in the binary mixtures of acetonitrile-propylene carbonate in the temperature range 298 K – 318 K. The interaction between acetonitrile and propylene carbonate molecules becoming stronger at 318 K than at 298 K.

3.2 ETHYL ACETATE – 2METHOXYETHANOL SYSTEM (EA-2ME)
In EA-2ME system, the variation of excess thermodynamic functions βs^E, L_f^E and V^E at all temperatures studied are shown in Figures 4-6. All these excess parameters show a negative deviation for the entire composition range of EA (X_1=0-1 mole fraction) and for the temperature range studied. The negative deviation of βs^E, L_f^E and V^E increases with increase of temperature showing maximum deviation at 323.15 K. The magnitude of negative deviation reaches a maximum at X_1=0.5463 mole fraction of EA and then becoming less and less negative with further increase in concentration of EA in 2ME.

The negative deviation of βs^E, L_f^E and V^E observed in EA-2ME system at all the temperatures studied is similar to that in MA-2ME system, so the explanation offered for MA-2ME system is equally applicable to EA-2ME system. The negative deviation of βs^E, L_f^E and V^E increases with increase of temperature reaching a maximum at 323.15 K. This indicates that the complex formation is much stronger at 323.15 K.

3.3 IR STUDIES
IR spectra are recorded for MA and EA in 2ME systems at 303.15 K are shown in figures 7 - 12. In MA-2ME system, these spectra were recorded at X_1 = 0.3983, 0.4983, 0.5983 molefraction of MA. The recorded spectra are shown in figures 7-9. In EA-2ME system, the spectra were recorded at X_1 = 0.4453, 0.5463, 6520 molefraction of EA. These spectra are shown in figures 10–12. In all the spectra recorded, a broad absorption band centered around 3500 cm^{-1} is observed. This indicates the presence of intermolecular hydrogen bonding between MA and 2ME molecules of this system [26].

In MA-2ME system, a broad absorption band occurs at 3496 cm^{-1}, 3425 cm^{-1} and 3512 cm^{-1} respectively, corresponding to X_1= 0.3983, 0.4983 and 0.5983 molefraction of MA (figures 7-9). In EA-2ME system, a broad absorption band occurs at 3523 cm^{-1}, 3457 cm^{-1} and 3532 cm^{-1} respectively, corresponding to X_1= 0.4453, 0.5463, 6520 molefraction of EA (figures 10–12). The broad band observed at 3496 cm^{-1} for

X_1=0.3983 molefraction of MA shifts towards the lower frequency side by 81 cm^{-1}, when X_1 is increased from 0.3983 to 0.4983 molefraction. But for X_1 = 0.5983 molefraction, the broad absorption band shifts towards higher frequency side and occurs at 3512 cm^{-1}. Among the three concentrations of MA, the maximum lower frequency shift is observed at X_1=0.4983 molefraction of MA, thus showing that the association through intermolecular hydrogen bonding is stronger at this concentration [26]. This confirms our excess compressibility and excess molar volume studies carried out in 2ME-MA system. The IR spectra recorded for 2ME-EA system also exhibits a similar behaviour as that of 2ME-MA system. Hence the explanation offered for the IR spectra of 2ME-MA systems also holds good for 2ME-EA system.

IV. Conclusion

The excess thermodynamic functions such as βs^E, L_f^E and V^E are calculated for the binary mixtures of methyl acetate-2methoxyethanol and ethyl acetate-2 methoxyethanol in the temperature range 303.15 K – 323.15 K. All these parameters show negative deviation in the composition range X_1= 0-1 mole fraction of methyl acetate and ethyl acetate in 2-methoxyethanol and at all the temperatures studied. Both the binary mixtures show a maximum negative deviation at 323.15 K indicating that the complex formation is much stronger at this temperature. In the binary mixtures studied, the formation of complexes is due to the formation of hydrogen bonding between the oxygen of carbonyl group (C=O) of methyl acetate, ethyl acetate with the hydroxyl group (OH) of 2-methoxyethanol. The formation of intermolecular hydrogen bonding between the components of liquid mixtures in the present study has been confirmed by recording of IR spectra of pure liquids and liquid mixtures.

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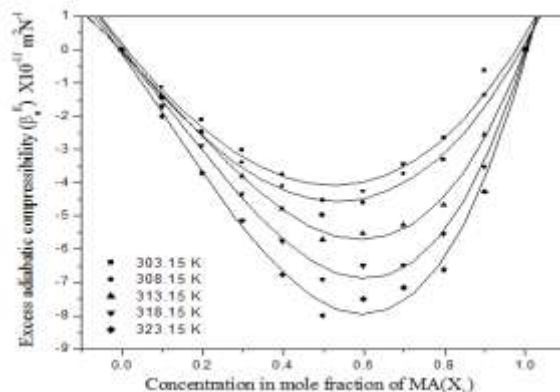
Figure: 1 Variation of excess adiabatic compressibility (β_s^E) with concentration in mole fraction (x_1) for MA-2ME system at temperatures between (303.15 and 323.15) K. 303.15 K :■, 308.15 K : ● , 313.15 K : ▲, 318.15 K : ▼, 323.15 K : ♦.

Figure: 2 Variation of excess free length (L_f^E) with concentration in mole fraction(x_1) for MA-2ME system at temperatures between (303.15 and 313.15) K. 303.15 K :■, 308.15 K : ● , 313.15 K : ▲, 318.15 K : ▼, 323.15 K : ♦.
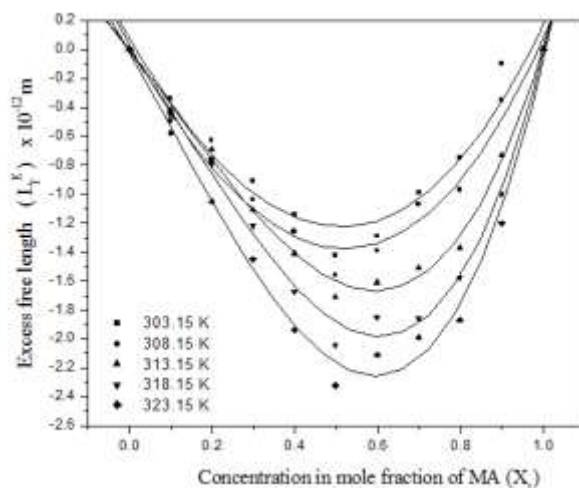

Figure :3 Variation of excess molar volume (V^E) with concentration in mole fraction (x_1) for MA-2ME system at temperatures between(303.15 and 323.15) K. 303.15 K :■, 308.15 K : ● , 313.15 K : ▲, 318.15 K : ▼, 323.15 K : ♦.
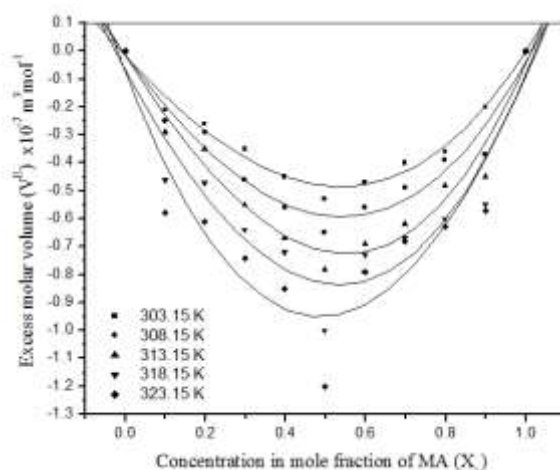

Figure :4 Variation of excess adiabatic compressibility (β_s^E) with concentration in mole fraction (x_1) for EA-2ME system at temperatures between(303.15 and 323.15)K. 303.15 K :■,308.15 K : ●, 313.15 K : ▲, 318.15 K : ▼, 323.15 K : ♦.

Figure: 5 Variation of excess free length (L_f^E) with concentration in mole fraction (x_1) forEA-2ME system at temperatures between(303.15 and 323.15) K. 303.15 K :■, 308.15 K : ● ,313.15 K : ▲, 318.15 K : ▼, 323.15 K : ♦.
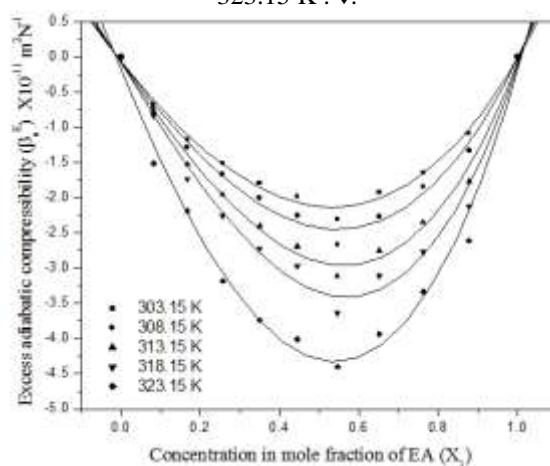

Figure :6 Variation of excess molar volume (V^E) with concentration in mole fraction (x_1) for EA-2ME system at temperatures between (303.15 and 323.15) K. 303.15 K :■, 308.15 K :●, 313.15 K : ▲, 318.15 K : ▼, 323.15 K : ♦.
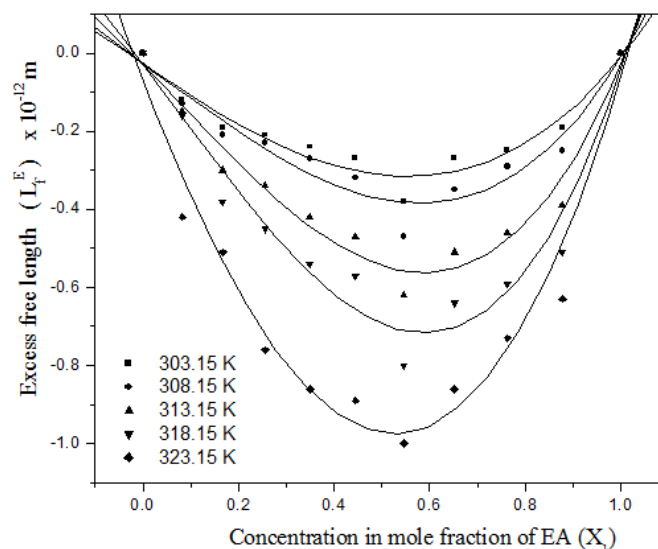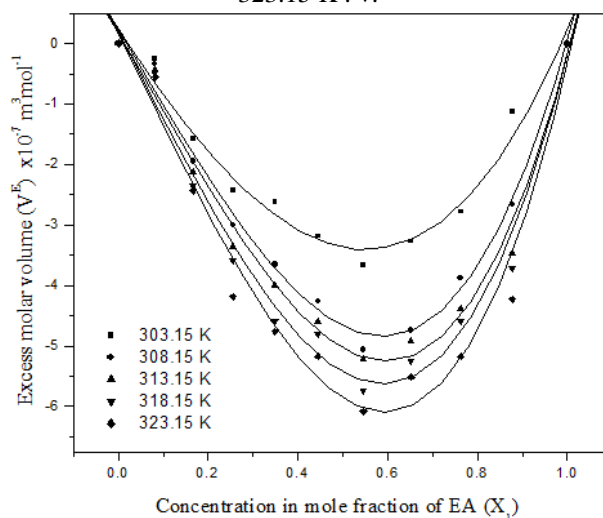

FIGURE 7 – FTIR spectrum for X_1=0.3983 molefraction of methyl acetate for 2ME-MA system at 303.15 K.

FIGURE 8 – FTIR spectrum for X_1=0.4983 molefraction of methyl acetate for 2ME-MA system at 303.15 K

FIGURE 9 – FTIR spectrum for X_1=0.5983 molefraction of methyl acetate for 2ME-MA system at 303.15 K.
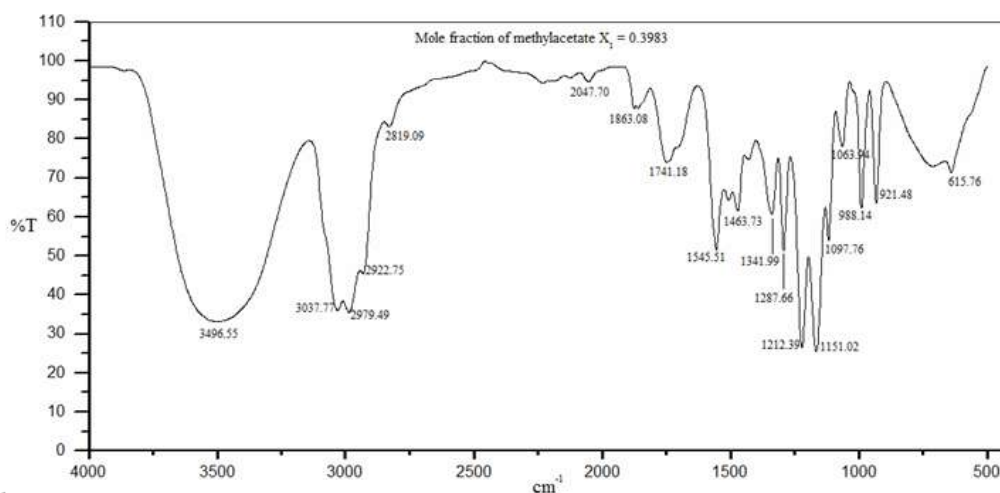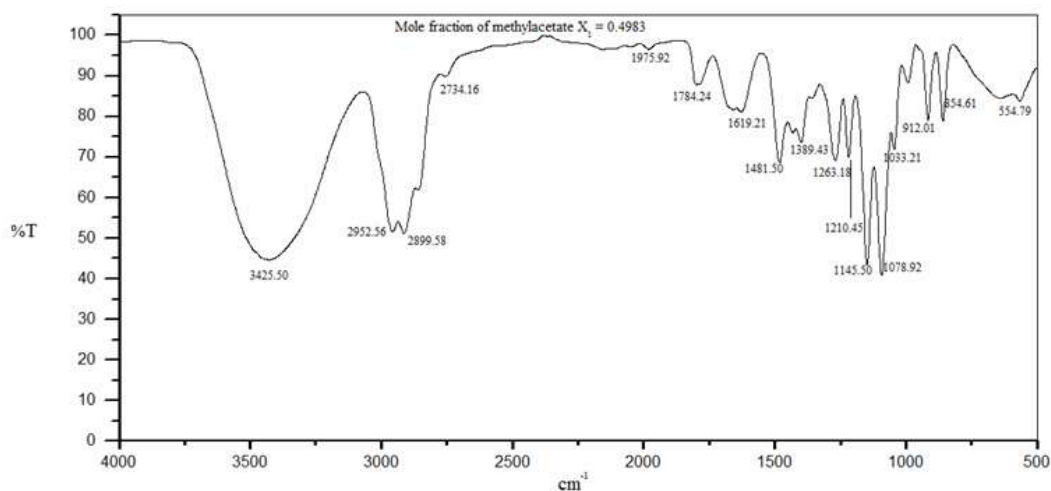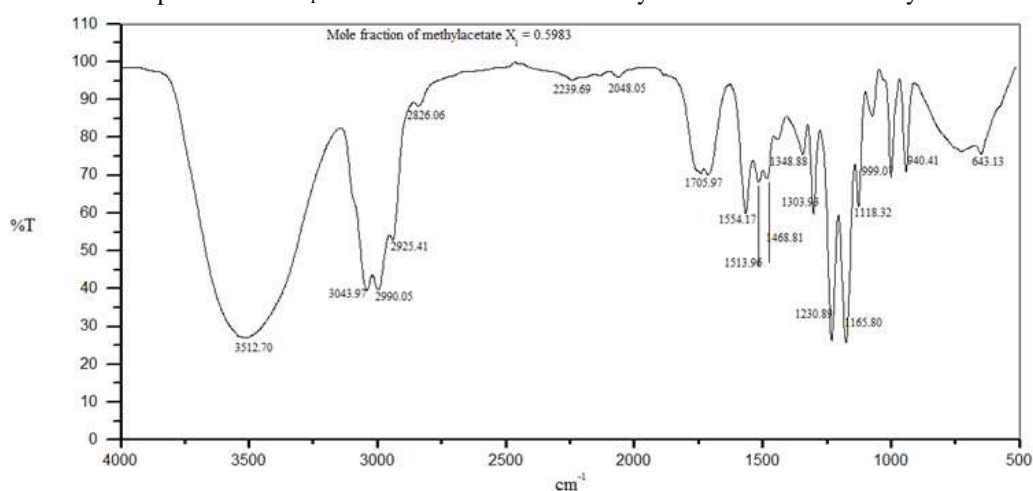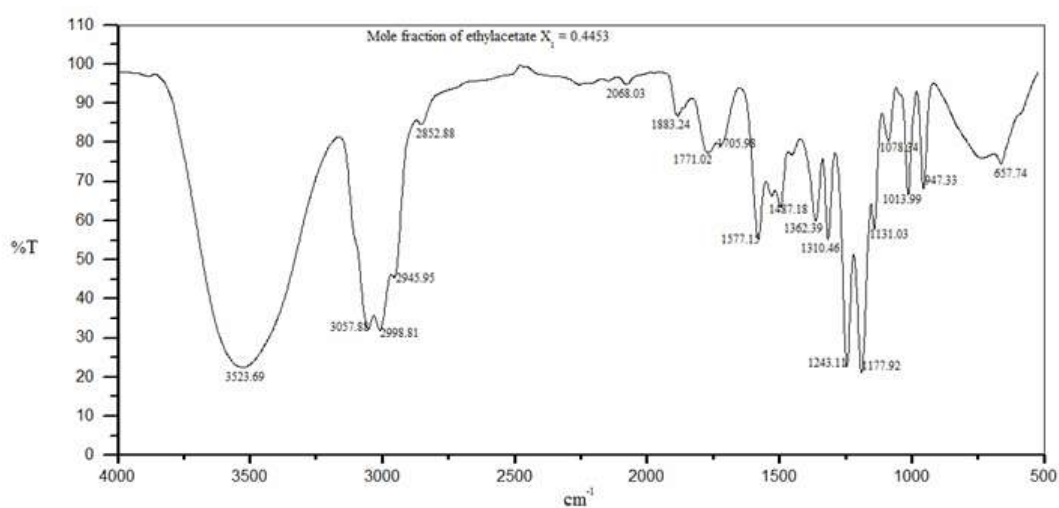

FIGURE 10 – FTIR spectrum for X_1=0.4453 molefraction of ethyl acetate for 2ME-EA system at 303.15 K.
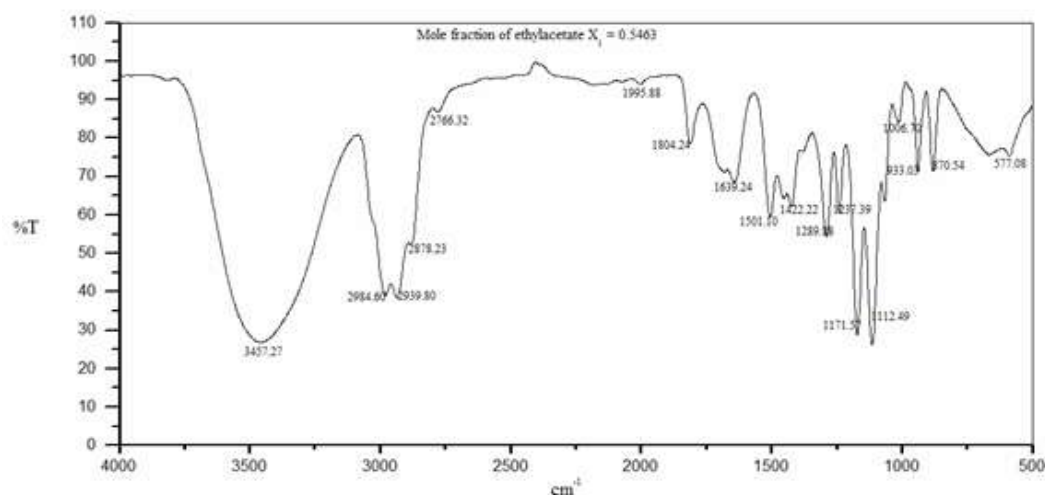
FIGURE 11 – FTIR spectrum for X_1=0.5463 molefraction of ethyl acetate for 2ME-EA system at 303.15 K
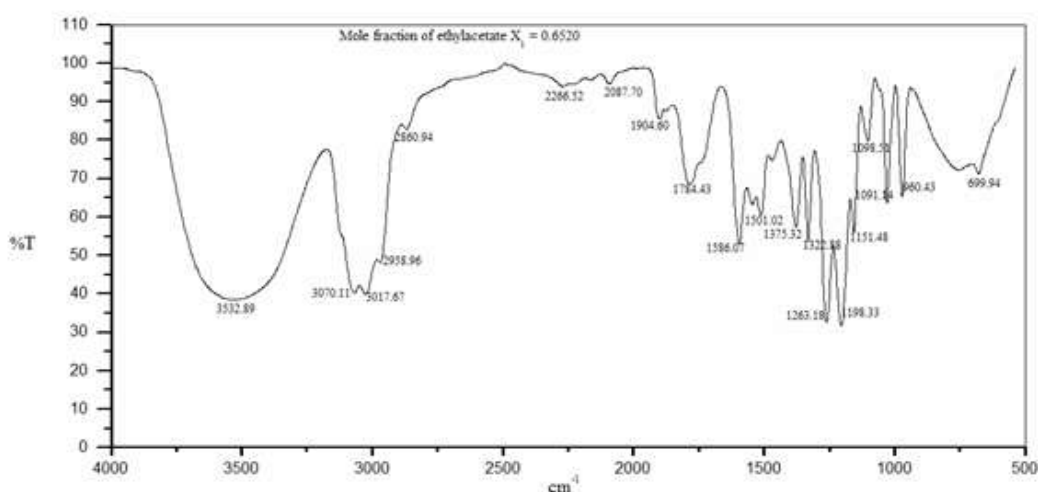

FIGURE 12 – FTIR spectrum for X_1=0.6520 molefraction of ethyl acetate for 2ME-EA system at 303.15 K.

Table 1 - Density values of pure 2-methoxyethanol (2ME), methyl acetate (MA) and ethyl acetate (EA)

Liquids	Density (g / cm^3)	
	Literature value (298.15 K)	Measured value (303.15 K)
2-Methoxyethanol (2ME)	0.965	0.963
Methyl acetate (MA)	0.932	0.930
Ethyl acetate (EA)	0.897	0.893

Table 2- Ultrasonic velocity (U) and density (ρ) of MA-2ME system at temperatures between (303.15 and 323.15)K.

X_1 Mole fraction	Velocity (U) (ms^{-1})					Density (ρ) (kgm^{-3})				
	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0	1417.51	1408.43	1379.15	1347.32	1320.15	963.54	941.52	912.96	889.13	866.35
0.099	1390.79	1384.34	1352.42	1320.77	1294.94	960.54	938.68	909.97	886.46	863.71
0.198	1363.99	1357.73	1323.06	1291.24	1268.98	957.34	935.61	906.73	883.34	860.54
0.298	1337.66	1330.94	1298.23	1265.76	1242.04	954.17	932.65	903.62	880.35	857.43
0.398	1311.08	1303.73	1271.83	1241.54	1218.37	951.01	929.62	900.42	877.27	854.32
0.497	1286.99	1279.95	1246.91	1216.95	1193.53	947.86	926.62	897.25	874.47	851.47
0.598	1254.01	1246.01	1214.05	1182.34	1158.72	944.49	923.35	893.81	870.97	847.83
0.698	1219.26	1211.01	1183.79	1153.57	1127.93	941.15	920.13	890.43	867.77	844.53
0.798	1187.69	1182.35	1153.50	1121.25	1098.65	937.84	916.89	886.98	864.56	841.28
0.899	1149.61	1145.10	1115.99	1085.56	1062.32	934.37	913.71	883.63	861.35	838.01
1	1124.29	1115.17	1079.97	1046.14	1021.27	930.85	910.15	879.84	857.65	834.26

X_1-Mole fraction of Methyl acetate

X_1 Mole fraction	Velocity (U) (ms^{-1})					Density (ρ)(kgm^{-3})				
	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0	1417.23	1406.72	1378.32	1349.74	1321.51	963.36	942.02	913.44	890.21	868.24
0.082	1389.43	1377.98	1350.59	1323.28	1300.28	956.66	935.73	908.51	886.32	864.95
0.167	1359.28	1346.72	1321.91	1296.91	1270.61	951.21	930.85	904.89	883.77	862.89
0.256	1328.14	1314.71	1290.87	1267.71	1244.17	945.11	925.25	900.68	880.51	860.61
0.349	1298.02	1283.68	1261.33	1238.84	1215.43	938.23	919.14	895.79	876.93	857.14
0.445	1268.02	1253.32	1231.73	1209.96	1185.88	931.82	913.02	890.87	872.59	853.53
0.546	1239.88	1224.92	1203.85	1184.33	1157.53	925.23	907.03	885.89	868.86	850.28
0.652	1207.43	1191.76	1171.62	1151.95	1125.59	917.71	899.87	879.99	863.78	845.71
0.763	1177.33	1160.32	1140.77	1122.32	1094.32	910.14	892.24	873.89	858.54	841.32
0.878	1147.51	1130.32	1110.74	1092.63	1064.44	901.58	884.42	867.53	853.21	836.49
1	1115.15	1097.43	1076.65	1057.93	1028.72	893.53	875.32	859.02	845.53	829.06

Table 3 - Ultrasonic velocity (U) and density (ρ) of EA-2ME system at temperatures between (303.15 and 323.15)K.

X_1-Mole fraction of ethyl acetate

Table 4 - The coefficients of Redlich-Kister equation computed for βs^E, L_f^E and V^E by least square fit method along with the standard deviations (σ) for
MA – 2ME system at temperatures between (303.15 and 323.15) K.
Coefficients X 10^{11} of equation (βs^E / $X_1 X_2$)=[A_0 + $A_1(2X_1-1)$+$A_2(2X_1-1)^2$+$A_3(2X_1-1)^3$]
for excess adiabatic compressibility (βs^E)in m^{2}N^{-1}

Temp	A_0	A_1	A_2	A_3	σ 10^{-11} m^{2}N^{-1}
303.15 K	-17.65	-6.55	11.35	15.23	1.26
308.15 K	-18.68	-5.45	4.75	8.49	1.39
313.15 K	-21.88	-10.78	-0.48	4.52	1.11
318.15 K	-25.64	-12.21	-4.16	-0.67	1.38
323.15 K	-29.56	-10.90	-7.60	-7.45	1.61

Coefficients X 10^{12} of equation (L_f^E / $X_1 X_2$)=[A_0 + $A_1(2X_1-1)$+$A_2(2X_1-1)^2$+$A_3(2X_1-1)^3$]
for excess freelength (L_f^E) in m

Temp	A_0	A_1	A_2	A_3	σ 10^{-12} m
303.15 K	-5.42	-1.95	4.36	5.51	0.46
308.15 K	-5.72	-1.50	1.86	3.28	0.55
313.15 K	-6.42	-3.21	0.12	1.45	0.44
318.15 K	-7.43	-3.73	-1.04	0.12	0.55
323.15 K	-8.46	-2.96	-2.09	-2.25	0.61

Coefficients X 10^7 of equation (V^E / $X_1 X_2$)=[A_0 + $A_1(2X_1-1)$+$A_2(2X_1-1)^2$+$A_3(2X_1-1)^3$]
for excess molar volume (V^E) in m^{3}mol^{-1}

Temp	A_0	A_1	A_2	A_3	σ 10^{-7} m^{3}mol^{-1}
303.15 K	-1.93	-0.66	-0.65	1.03	0.22
308.15 K	-2.23	-0.02	-1.51	-1.26	0.45
313.15 K	-2.71	-0.12	-1.84	-1.52	0.52
318.15 K	-3.01	-0.18	-3.44	-0.73	0.84
323.15 K	-3.36	0.28	-4.06	-0.40	1.00

Table 5- The coefficients of Redlich-Kister equation computed for βs^E, L_f^E and V^E by least square fit method along with the standard deviations (σ) for
EA – 2ME system at temperatures between (303.15 and 323.15)K.
Coefficients X 10^{11} of equation (βs^E / $X_1 X_2$)=[A_0 + $A_1(2X_1-1)$+$A_2(2X_1-1)^2$+$A_3(2X_1-1)^3$] for excess adiabatic compressibility (βs^E)in m^{2}N^{-1}

Temp	A_0	A_1	A_2	A_3	σ 10^{-11} m^{2}N^{-1}
303.15 K	-8.26	-1.35	-1.95	0.66	0.51
308.15 K	-9.41	-1.90	-2.47	0.21	0.76
313.15 K	-11.17	-2.07	-4.02	-3.02	0.78
318.15 K	-12.75	-2.18	-5.04	-5.54	1.01
323.15 K	-16.13	-2.33	-8.50	-2.24	1.48

Coefficients X 10^{12} of equation (L_f^E / $X_1 X_2$)=[A_0 + $A_1(2X_1-1)$+$A_2(2X_1-1)^2$+$A_3(2X_1-1)^3$] for excess freelength (L_f^E) in m

Temp	A_0	A_1	A_2	A_3	σ 10^{-12} m
303.15 K	-1.18	-0.39	-0.74	0.42	0.20
308.15 K	-1.39	-0.58	-0.89	0.30	0.26
313.15 K	-2.01	-0.53	-1.36	-0.92	0.29
318.15 K	-2.58	-0.48	-1.65	-1.84	0.37
323.15 K	-3.51	-0.46	-2.96	-0.22	0.55

Coefficients X 10^7 of equation (V^E / $X_1 X_2$)=[A_0 + $A_1(2X_1-1)$+$A_2(2X_1-1)^2$+$A_3(2X_1-1)^3$] for excess molar volume (V^E) in m^{3}mol^{-1}

Temp	A_0	A_1	A_2	A_3	σ 10^{-7} m^{3}mol^{-1}
303.15 K	-14.69	-1.51	9.30	-2.99	2.13
308.15 K	-19.15	-2.61	3.59	-14.60	1.79
313.15 K	-19.85	-0.90	-2.64	-24.23	1.50
318.15 K	-21.41	0.10	-2.82	-27.26	1.73
323.15 K	-22.74	0.63	-5.92	-32.68	1.69