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Ultrasonic Studies of Binary Liquid Mixtures: Ethyl Acetate + 2-Butanone

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ABSTRACT

Binary liquid mixtures of Ethyl acetate + 2-Butanone at various mole fractions were prepared. The molecular interactions between the binary mixtures were analyzed by ultrasonic measurements using interferometer method. The densities of pure liquid mixtures were elucidated by relative measurement method. The mole fractions of Ethyl acetate and 2-Butanone were found to be 98.50 and 98.06 respectively. The FTIR spectrum shows a drastic change in the frequency for 0.6 mole fraction of Ethyl acetate and 0.4 mole fraction of 2-Butanone. The shift in the frequency values might be due to interstitial accommodation or induced dipole interaction.

Keywords: Ethyl acetate, 2-Butanone, FTIR, ultrasonic measurements.

INTRODUCTION

Ion-solvent or solvent-solvent interaction involved in a binary mixture system can be studied by various methods. The principle of acoustics is one among them [1,2]. Studies on acoustic parameters have become an emerging hid in recent years [3,4]. To understand solution chemistry, it is essential to know the salvation behavior of binary mixture system. Acoustic parameters are sensitive to changes and are useful in elucidating the solvent-solvent interaction. Moreover the ultrasonic velocity measurements have been successfully employed to detect and assess weak and strong molecular interactions, present in binary and ternary. In prevailing literature, many contributions have been made in the strong of liquid mixtures [7-13]. Literature does not show any report on the ultrasonic behavior of Ethyl acetate + 2-Butonone. In the present paper, an attempt has been made to determine the densities and ultrasonic velocities of the above said title binary mixtures have been reported.

MATERIALS AND METHODS

Commercially available AR grade Ethyl acetate (E-merk) and 2-Butanone (E-merk) were used as such. Densities were measured with the help of bicapillary pyknometer. All the weighings were made using single pan digital balance. The binary mixtures were prepared by volume, by mixing selected □volumes of liquid components in airtight glass bottles. In all the property measurements, an INSREF thermostat was used at a constant digital temperature display accrete to (± 0.1mg) and the measurement of mass were made using an electronic balance. Accuracy of density measurement was 0.0001 gcm^{-3}. A set of eleven compositions was prepared for each system and their physical properties were measured on the same day. A 10 ml. specific gravity bottle and electronic balance were used for the determination of density measurements. Speed of sound was determined using constant frequency (2 MHz) variable path ultrasonic interferometer (Model F- 81, Mittal Enterprises, New Delhi) with an accuracy of ± **2** ms^{-1} and was calibrated using water and benzene.

RESULTS AND DISCUSSION

Ultrasonic Velocity Measurement

The velocity of ultrasonic waves in the mixture has been measured by Interferometer method. The interferometer consists of two parts namely high frequency generator and the measuring cell. The interferometer generates alternating field for variable frequencies. The frequency of the alternating field in the interferometer can be selected by changing the selector available on the front panel. Thus, alternating field of a fixed frequency is generated by the interferometer. The measuring cell is a double walled vessel with a provision to circulate water from the water bath between the inner and outer walls. Thus the temperature of the mixture (taken in the inner cell) can be kept constant. At the top of the cell, a fine micrometer screw is fitted with a (metal) reflector, which is immersed in the mixture. The reflector plate in the mixture can be raised or lowered through a know distance using a micrometer screw. The least count of the micrometer screw is 0.001 mm. A quartz crystal is mounted at the bottom of the cell. The reflector plate and the quartz crystal are parallel to each other. The alternating field from the generator is applied to the quartz crystal. Therefore, quartz crystal gets into resonant vibrations and hence generates longitudinal ultrasonic waves.

The longitudinal ultrasonic waves generated by the crystal pass through the mixture and get reflected at the surface of the parallel reflector place. If the distance between the plate and the crystal is exactly an integral multiple of half wavelength, standing waves are formed within the medium. This leads to acoustic resonance, resulting in a change of potential difference at the generator, which excites the quartz crystal. Thus, the anode current of the generator becomes maximum. The change in the anode current can be measured from the micro-ammeter fitted with the frequency generator. The distance‘d’ between the plate and crystal is slowly varied using the micrometer screw, resulting in a decrease in anode current. The micrometer screw is adjusted such that the anode current increases up to a maximum once again i.e., the needle in the ammeter complete one oscillation. By noting the initial and final position of the micrometer for n complete movements (maxima-minima-maxima) of the micro-ammeter needle, one can determine the distance (d) moved by the parallel reflector. The wavelength is calculated as,

$$\lambda = \frac{2d}{n} \tag{1}$$

Therefore, the velocity of ultrasonic longitudinal waves in the mixture is given by,

$$U = \lambda f \tag{2}$$

Where, f is the frequency of the generator, which is used to excite the crystal.

Error Analysis

Let U_{expt} *and* U_{cal} be the experimental and theoretically calculated values of ultrasonic velocities

Percentage Deviation

The percentage deviation in the values of ultrasonic velocity is given by,

$$Percentage\ deviation = \frac{U_{expt} - U_{cal}}{U_{expt}} X\ 100 \tag{3}$$

Molecular Interaction Parameter

The Molecular Interaction Parameter (MIP) is given by,

$$MIP = \left(\frac{U_{cal}}{U_{exp}}\right)^2 - 1 \tag{4}$$

This MIP is multiplied by 100 for convenience of presentation of values.

Chi- Square value

Chi- square test of goodness of fit enables us to find whether the deviations of the theoretical values from the experimental ones are due to chance or really due to the inadequacy of the theory to fit the experimental data. χ^2 Value is given by,

$$\chi^2 - \sum_{i=1}^{n} \frac{(U_{expt} - U_{cal})^2}{U_{cal}} \tag{5}$$

Determination of Mole fraction

The Mole Fractions for Liquid-1 [Ethyl Acetate] and Liquid-2 [2-Butanone] are calculated as following as

Step 1: *To find the Mass of the water*

Mass of the empty R.D bottle (m_1) = 18.8701g
Mass of the water +R.D bottle (m_2) = 28.7041g
Therefore, Mass of the water alone (M) is M= (m_2-m_1) = 9.8340g

Step 2: *To find the Mass of the Liquid 1*

Mass of the empty R.D bottle (l_1) = 18.8701g
Mass of the Liquid 1 + R.D bottle (l_2) = 27.6804g
Therefore, Mass of the Liquid 1 alone (L_1) is L_1= (l_2-l_1) = 8.8103g

Step 3: *To find the Mass of the Liquid 2*

Mass of the empty R.D bottle (l'_1) = 15.1564g
Mass of the Liquid 1 + R.D bottle (l'_2) = 22.3990g
Therefore, Mass of the Liquid 1 alone (L_2) is L_2 = (l'_2-l'_1) = 7.2426g

Relative Density Formulae:

R.D.= [Mass of the liquid/ Mass of the water]X ρ_w (6)
Where, ρ_w is density of water.

Note: Density of water(ρ_w) = 1000 Kg/m^3 but, we take the approximate value of 0.9984 Kg/m^3.

Step 4: *To find the Density of the Liquid 1*
D_1= [Mass of the liquid 1/ Mass of the water]X ρ_w

Therefore,
D_1= [8.8103/ 9.8340]X 0.9984
D_1 = 0.8944 Kg/m^3

Step5: *To find the Density of the Liquid 2*

D_2= [Mass of the liquid 2/ Mass of the water]X ρ_w

Therefore,
D_2= [7.2426/ 9.8340]X 0.9984
D_2 = 0.7353Kg/m^3

Step 6: *To find the Molecular weight of the liquids*
Molecular weight of the Liquid 1 (MW_1) = 88.10 g/mol
Molecular weight of the Liquid 2 (MW_2) = 72.11 g/mol

Step 7: *To find the Mole Fraction*

The Mole Fraction for Liquid1 (MF_1) is calculated as-

MF_1= [MW_1/D_1]= [88.10/0.8944] = 98.5017

The Mole Fraction for Liquid2 (MF_2) is calculated as-
MF_2= [MW_2/D_2]= [72.11/0.7353] = 98.0688

The result of MF_1 and MF_2 are divided by 2 and 3

FTIR Spectrum Analysis

The FTIR spectrum of the binary mixtures was recorded in the frequency range 400-4000 cm^{-1} employing Broker model IFS 66V FTIR spectrometer. The spectra are shown in Fig. (1-11). The various frequency assignments pertaining to different ratios are tabulated in Table1.

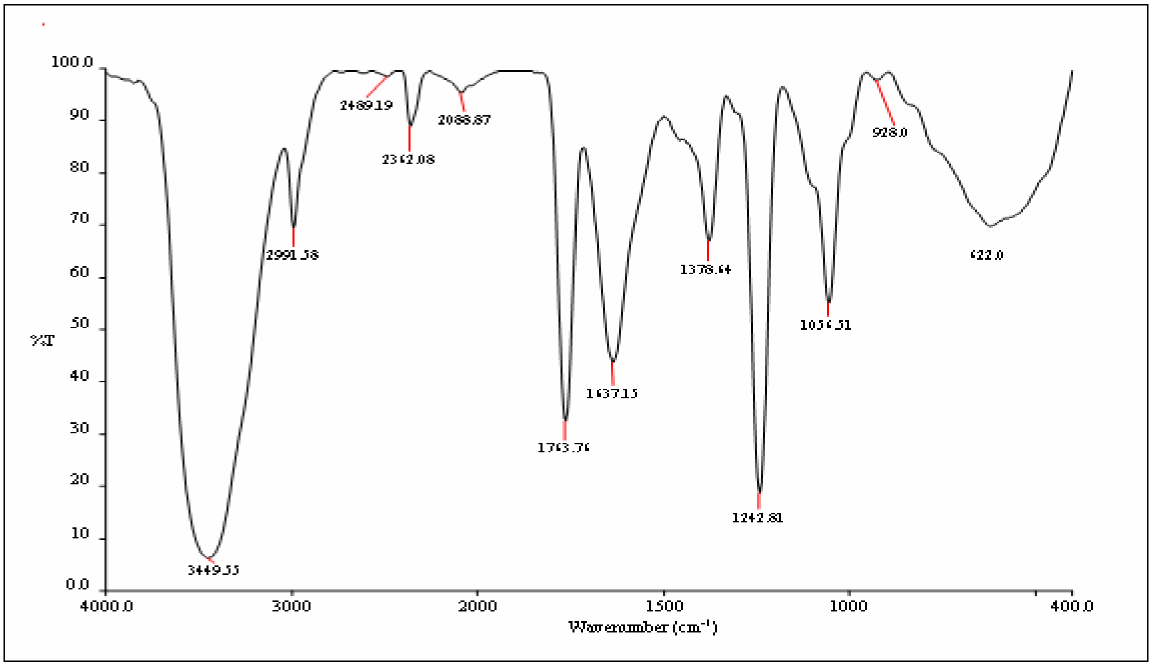
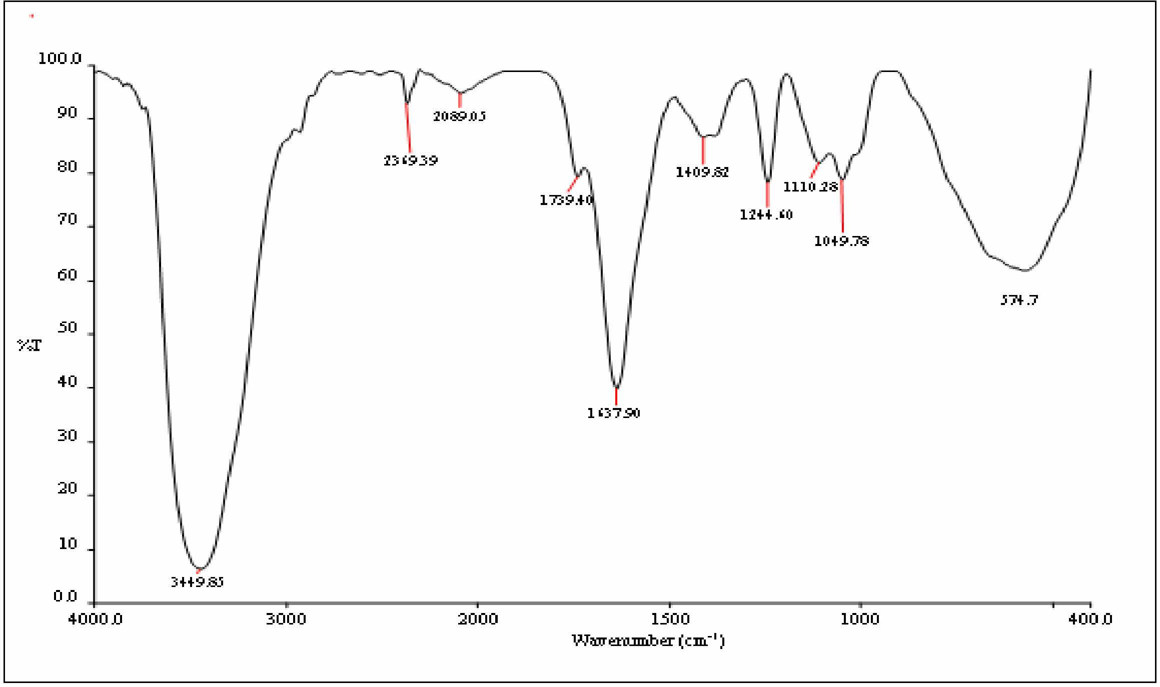


Fig.1



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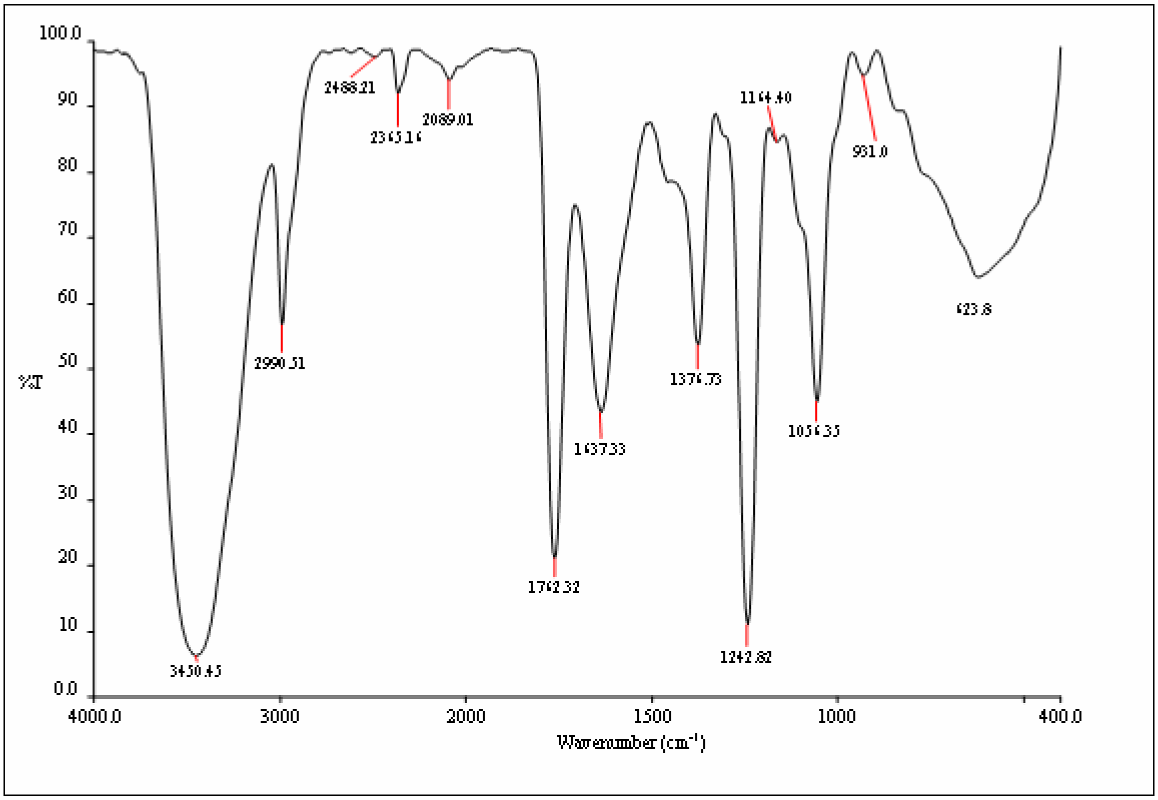
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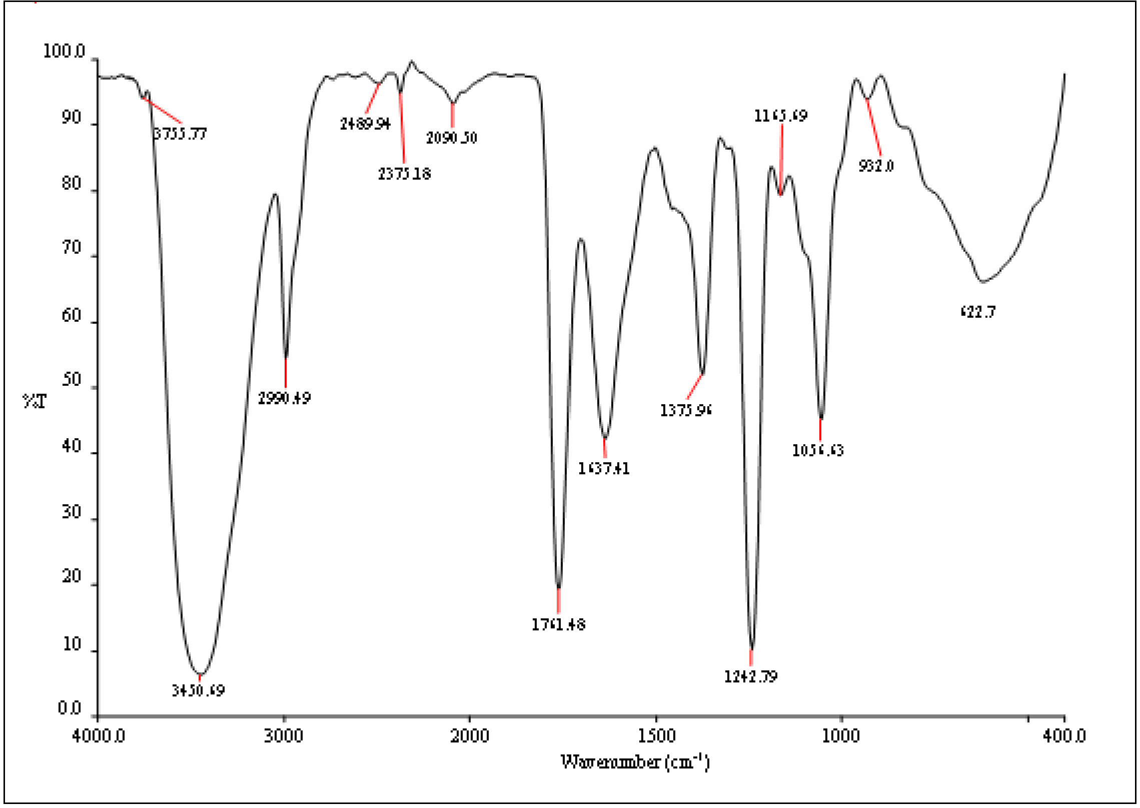
90
80
70
60
50
40
30
20
10
0.0
%T
4000.0
3000
2000
1500
1000
400.0
Wavenumber (cm⁻¹)
2488.21
2345.16
2089.01
2990.51
3450.45
1762.32
1637.33
1376.73
1164.40
1242.82
1056.35
931.0
623.8

Fig.3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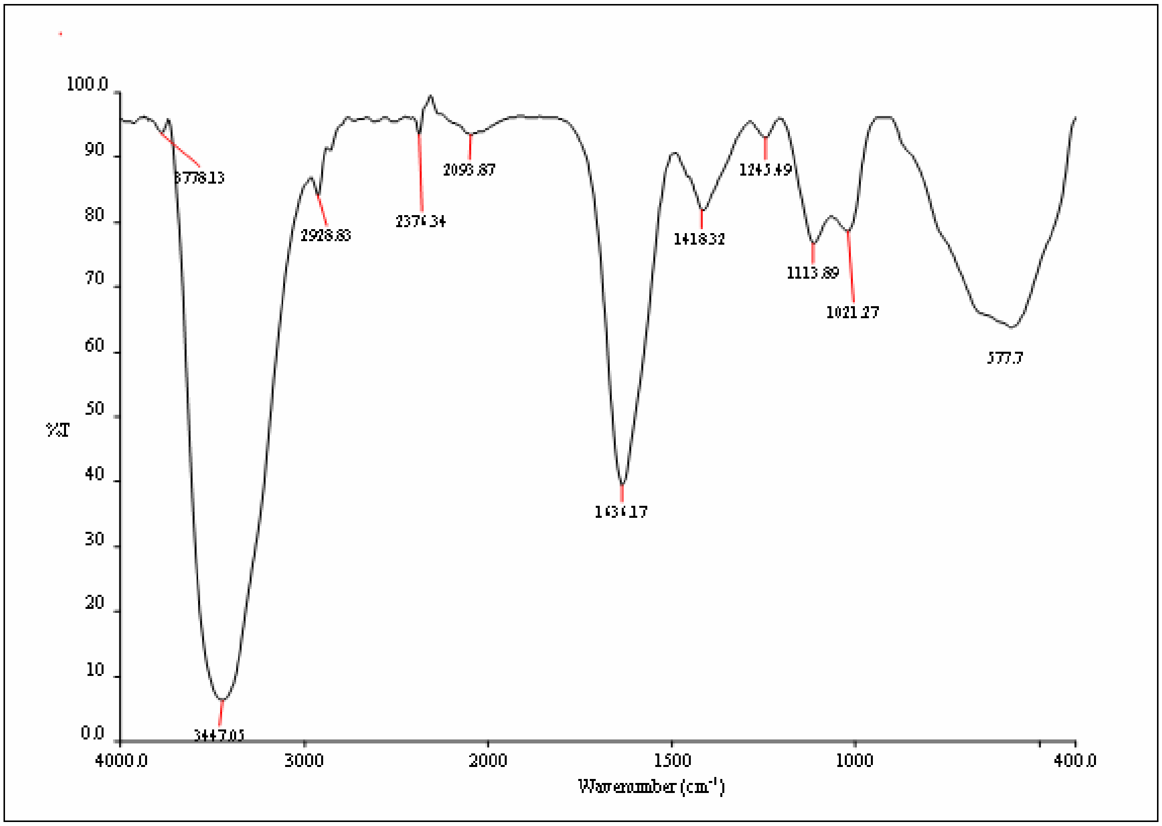
80
70
60
50
40
30
20
10
0.0
%T
4000.0
3000
2000
1500
1000
400.0
Wavenumber (cm⁻¹)
3755.77
2489.94
2375.18
2090.50
2990.49
3450.69
1761.48
1637.41
1375.96
1165.69
1242.79
1056.63
932.0
622.7

Fig.4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70
60
50
40
30
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10
0.0
%T
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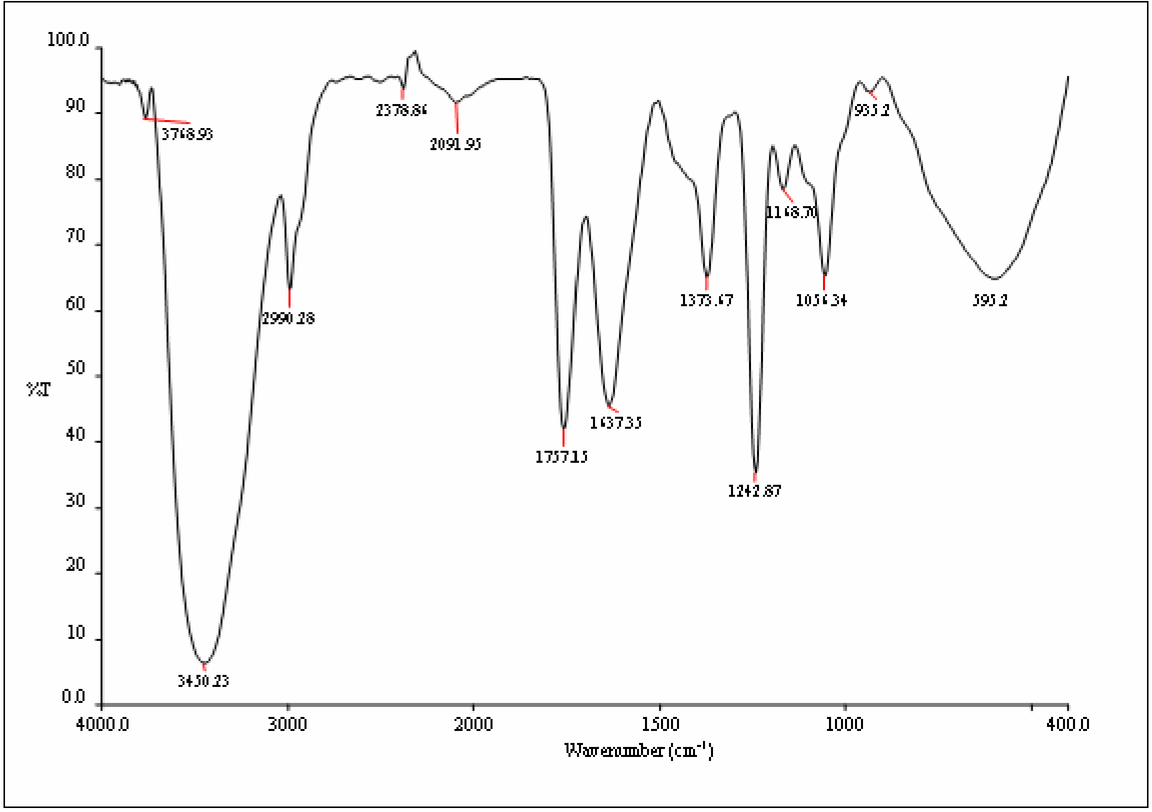
2093.87
1418.32
1245.49
1113.89
1021.27
577.7
1634.17
3447.05
4000.0
3000
2000
1500
1000
400.0
Wavenumber (cm-1)

Fig.5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60
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40
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1168.70
2990.28
1373.67
1054.34
595.2
1637.35
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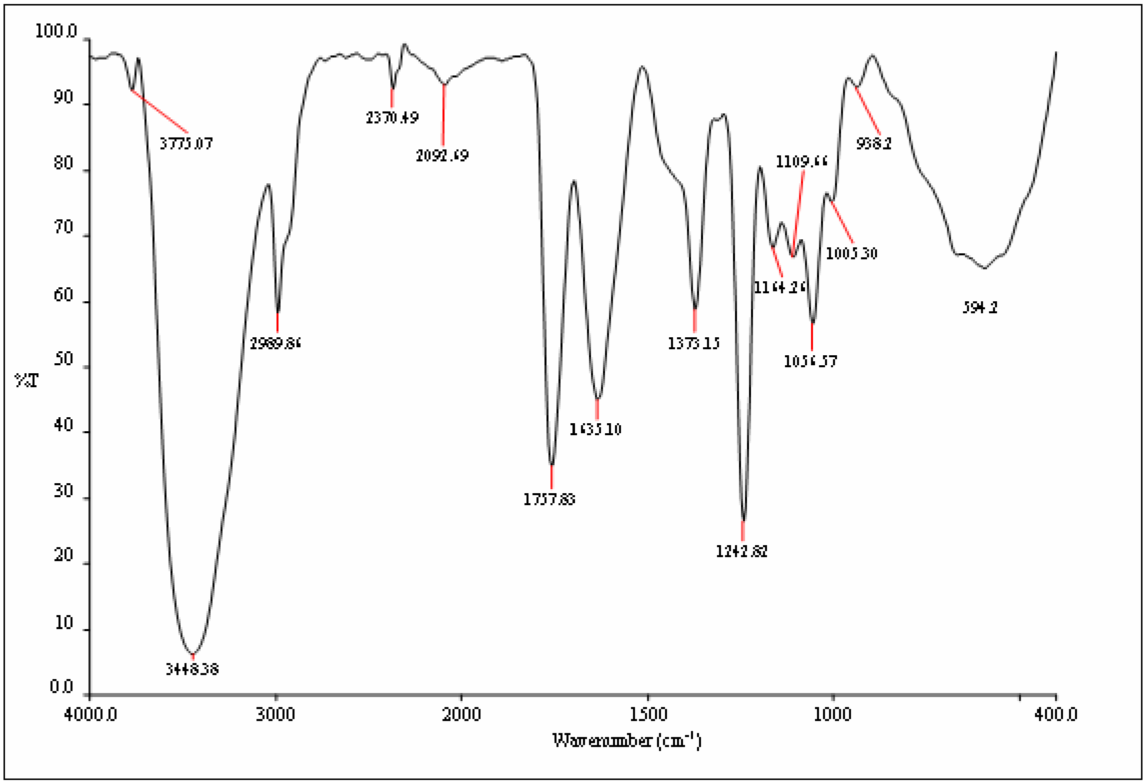
3000
2000
1500
1000
400.0
Wavenumber (cm-1)

Fig.6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60
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40
30
20
10
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%T
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2989.86
3448.38
1757.83
1635.10
1373.15
1242.82
1164.26
1109.66
1056.57
1005.30
938.2
594.2
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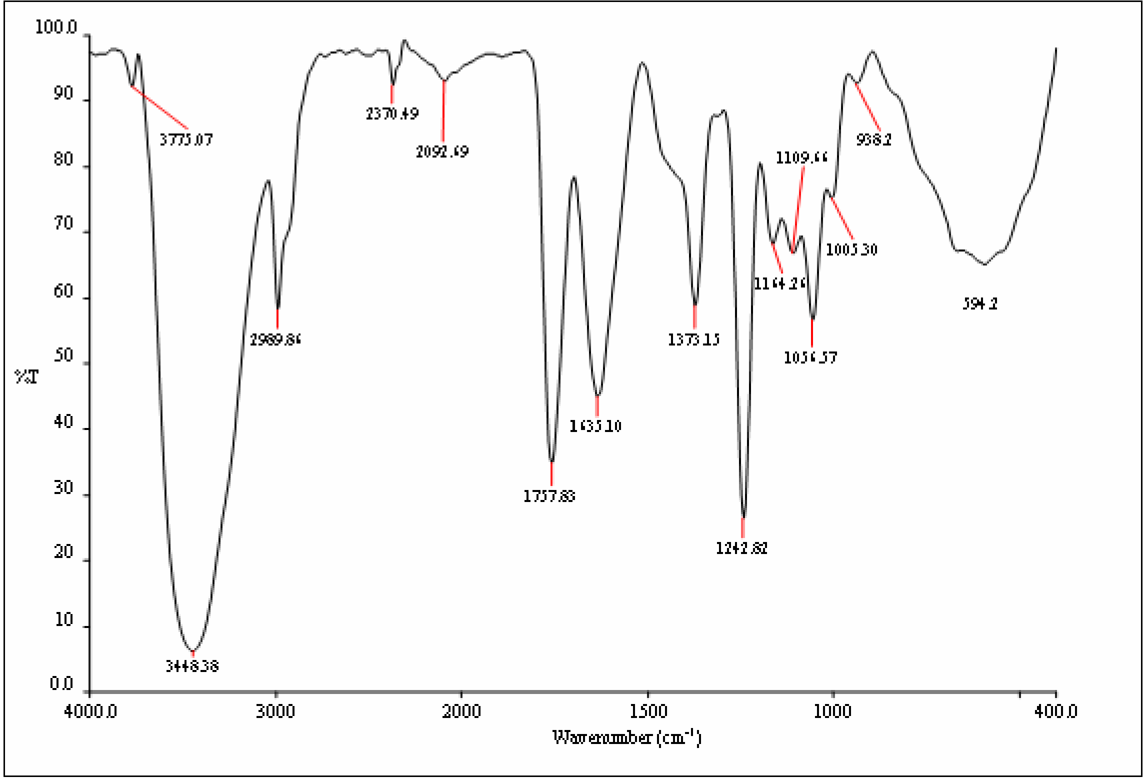
3000
2000
1500
1000
400.0
Wavenumber (cm^{-1})

Fig.7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70
60
50
40
30
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10
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%T
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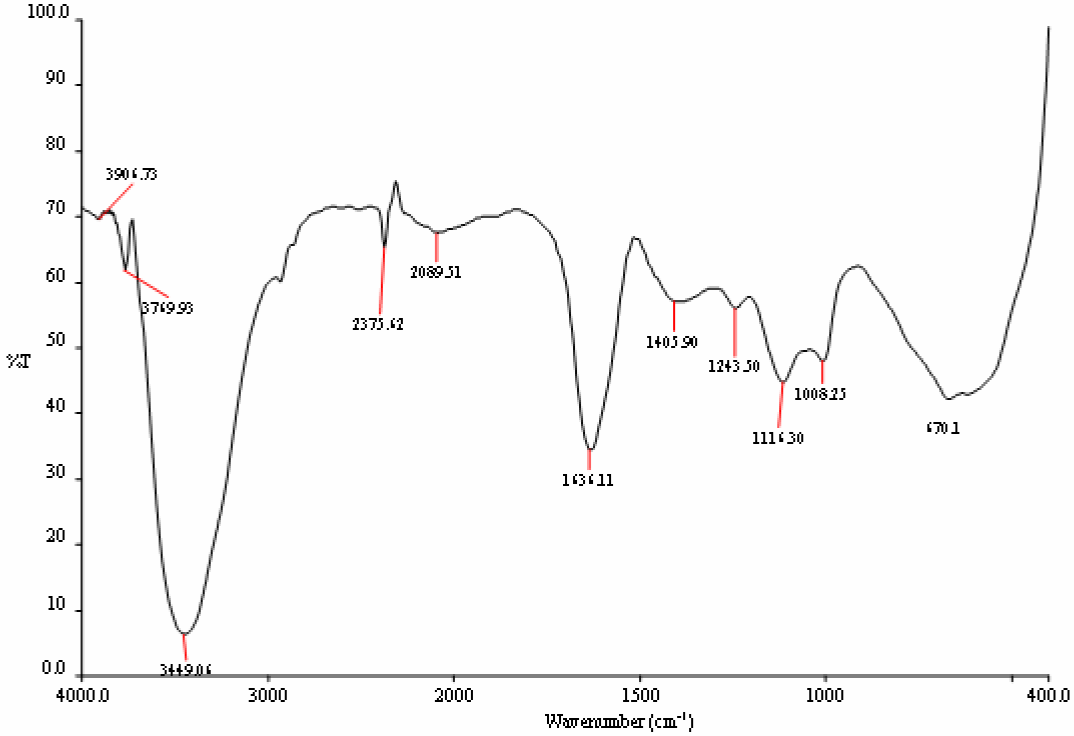
2989.86
3448.38
1757.83
1635.10
1373.15
1242.82
1164.26
1109.66
1056.57
1005.30
938.2
594.2
4000.0
3000
2000
1500
1000
400.0
Wavenumber (cm^{-1})

Fig.8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90
80
70
60
50
40
30
20
10
0.0
%T
3906.73
3769.93
3449.06
2375.62
2089.51
1636.11
1405.90
1243.50
1116.30
1008.25
670.1
4000.0
3000
2000
1500
1000
400.0
Wavenumber (cm⁻¹)

Fig.9

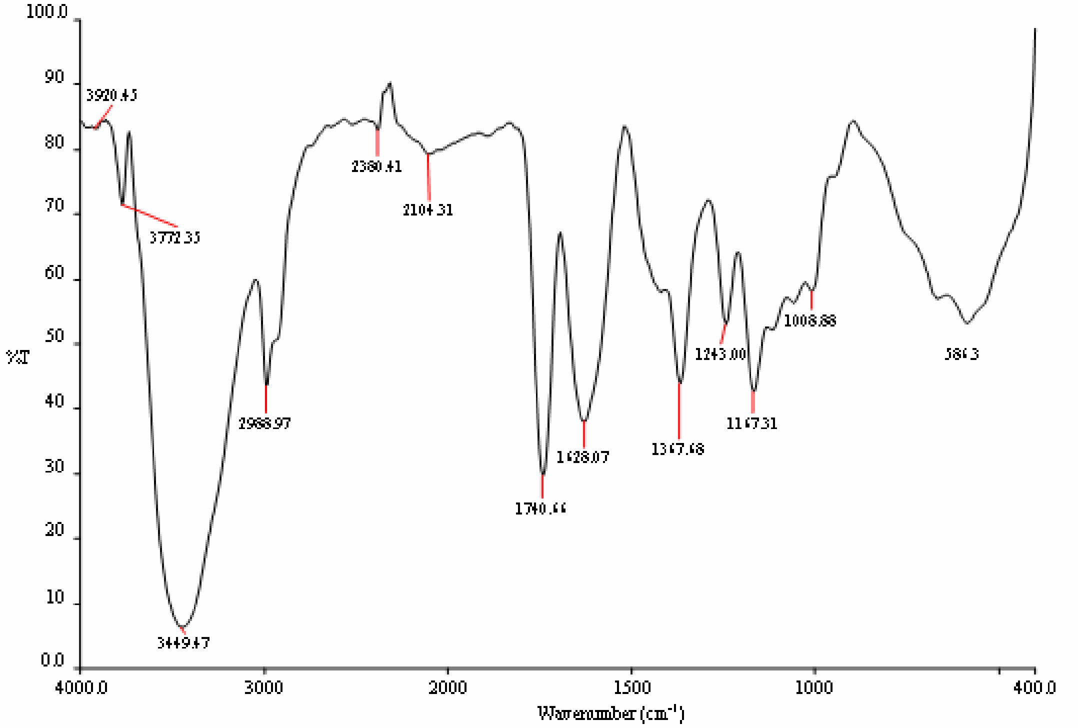
100.0
90
80
70
60
50
40
30
20
10
0.0
%T
3920.45
3772.35
3449.47
2968.97
2380.41
2104.31
1740.66
1628.07
1367.68
1243.00
1167.31
1008.88
586.3
4000.0
3000
2000
1500
1000
400.0
Wavenumber (cm⁻¹)

Fig.10

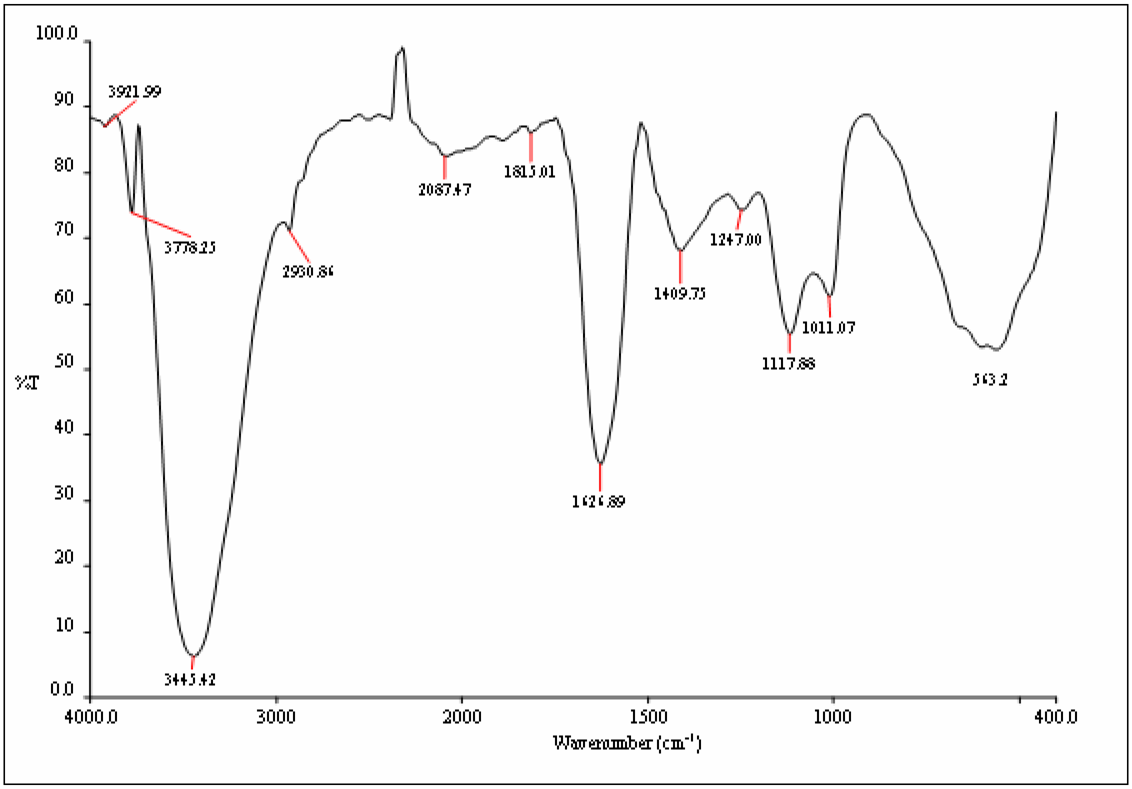

Fig.11

Observations of FTIR Spectrum

Table-1

1 (EA) + 0.0 (2BUT)	0.9 (EA) + 0.1 (2BUT)	0.8 (EA) + 0.2 (2BUT)	0.7 (EA) + 0.3 (2BUT)	0.6 (EA) + 0.4 (2BUT)	0.5 (EA) + 0.5 (2BUT)	0.4 (EA) + 0.6 (2BUT)	0.3 (EA) + 0.7 (2BUT)	0.2 (EA) + 0.8 (2BUT)	0.1 (EA) + 0.9 (2BUT)	0 (EA) + 1 (2BUT)
3449.55	3449.85	3450.45	3755.77	3778.13	3768.93	3775.07	3765.76	3906.73	3920.45	3921.99
2991.58	2369.39	2990.51	3450.69	3447.05	3450.23	3448.38	3448.32	3769.93	3772.35	3778.25
2489.19	2089.05	2488.21	2990.49	2928.83	2990.28	2989.86	2988.64	3449.06	3449.47	3445.42
2362.08	1739.40	2365.16	2489.94	2376.34	2378.86	2370.49	2368.72	2375.62	2988.97	2930.86
2088.87	1637.90	2089.01	2375.18	2093.87	2091.95	2092.69	2094.28	2089.51	2380.41	2087.47
1763.76	1409.82	1762.32	2090.50	1636.17	1757.15	1757.83	1746.98	1636.11	2104.31	1815.01
1637.15	1244.60	1637.33	1761.48	1418.32	1637.35	1635.10	1635.26	1405.90	1740.66	1626.89
1378.64	1110.28	1376.73	1637.41	1245.49	1373.67	1373.15	1370.94	1243.50	1628.07	1409.75
1242.81	1049.78	1242.82	1375.96	1113.89	1242.87	1242.82	1242.92	1116.30	1367.68	1247.00
1056.51	574.78	1164.40	1242.79	1021.27	1168.70	1164.26	1114.23	1008.25	1243.00	1117.88
928.00		1056.35	1165.69	577.76	1056.34	1109.66	595.48	670.17	1167.31	1011.07
622.08		931.02	1056.63		935.24	1056.57			1008.88	563.25
		623.89	932.09		595.26	1005.30			586.32	
			622.77			938.26				
						594.26				

CONCLUSION

In the case of Ethyl acetate + 2-Butanone mixture, the V^E is maximum negative for 0.6 mole fraction of Ethyl acetate which shows the presence of interstitial accommodation of one type of molecule into other and dipole – induced dipole interaction. The FTIR spectrum taken shows a drastic change in the frequency values for 0.6 mole fraction of Ethyl Acetate (0.6 of Ethyl Acetate and 0.4 of 2-Butanone). So, the observation from the V^E study has been confirmed by the FTIR spectrum measurement.The shift in the frequency values of FTIR spectrum measurement is generally due to following observed factors:

1. Interstitial accommodation.
2. Strong interactions (H- bond type, or dipole – dipole or dipole – induced dipole interactions).

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