

Volumetric, Ultrasonic and Infra-red Spectroscopic Study of Binary Liquid Mixture of o-xylene, m-xylene and p-xylene with t-butanol at 303.15 K

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Abstract: *Density, speed of sound, IR of binary mixture of o-xylene, m-xylene, p-xylene with t-butanol have been measure at 303.15 K. The excess molar volume (V^E) and excess Isentropic compressibility K_S^E have been calculated from the experimental value.*

The experimental sound velocity data have been analysed in terms of free length theory (FLT) and collision factor theory (CFT). The experimental result are discussed in terms of intermolecular interaction between unlike molecules

Keywords: *Density, Excess molar volume, ultrasonic velocity, Isentropic Compressibilities, FLT, CFT, I.R. Redlich-kister equation.*

1. INTRODUCTION

A survey of the literature shows that V^E data for the binary mixture of xylene with isoalcohols (1), xylene with esters (2), xylenes with aliphatic hydrocarbons (3) have been reported. Further V^E data for a series of 1-alkanols with xylenes at 298.15 K were also reported earlier (4-5). The present work was undertaken with view of utilizing this data for further study of excess thermodynamic properties at this temperature. Isentropic compressibilities data for binary mixture of o-xylene with 1-alkanols (6) were also reported earlier, the sound velocities in binary liquid mixture can be computed theoretically at different mole fractions from Jacobson's free length theory (7) (FLT) and collision factor theory (8) (CFT) of Shaff's. Both the theories have been successfully applied to binary mixture by many works (9-11). IR studies (12) of the mixture of ethyl iodide and ethyl alcohol benzene, toluene, o-xylene and p-xylene were carried out. IR spectral studies support the conclusion drawn.

2. EXPERIMENTAL

All the chemicals were used of analytical grade. t-butanol and xylenes were purified by the methods described by Reddick and Bunger (13). The purities of samples were checked by comparing the densities of the component with those reported in literature (14-20). Densities were determined using a bicapillary type pycnometer. Density values were reproducible within $\pm 5 \times 10^{-5} \text{ g cm}^{-3}$. Excess volumes were measured using the dilatometer of the type described earlier (21). Isentropic compressibilities (K_S) were computed from measured sound velocity data and density evaluated from excess volume.

The ultrasonic velocity was measured with a single crystal interferometer at 2 MHz frequency and the data were accurate to $\pm 0.15\%$ (using Mittal's F-81 model). FTIR spectra were recorded on a FTIR spectrometer (model SHIMADZU 8400 PC) by using KBr pellet in the region $4000-400 \text{ cm}^{-1}$ ($30 - 2.5 \mu\text{m}$).

3. RESULTS AND DISCUSSION

The experimental excess volume of three binary mixture are given table 1. V^E values were fitted to an empirical relation proposed by Redlich-kister

$$V^E = (x_1 M_1 + x_2 M_2)/\rho_{12} - (x_1 M_1/\rho_1) - (x_2 M_2/\rho_2) \quad (1)$$

where M_1 , x_1 , ρ_1 and M_2 , x_2 , ρ_2 are molecular weight, mole fraction and density of components 1 and 2 respectively of binary mixtures, ρ_{12} is the mixture density.

The values of the constant are given in the Table-2 along with standard deviation σ (V^E) data for density (ρ). Computed from measure are included in Table -3 Isentropic compressibility, K_S and deviation in isentropic compressibility, ΔK_S are also given in Table-3. The deviation in isentropic compressibility (ΔK_S) were calculated by using equation.

$$K_S = (1/u^2\rho) \quad (2)$$

$$\Delta K_S = K_{S12} - \phi_1 K_{S1} - \phi_2 K_{S2} \quad (3)$$

The sound velocity data predicted in terms of free length theory (FLT) and collision factor theory (CFT) are given along with experimental result in Table-4 However the velocity of sound predicted by FLT method are closer to experimental values.

The V^E data which is presented in Table-1 can be explained as follows. According to Treszezanowicz and Benson (22). The positive V^E values arises due to breaking of H-bonding in self association t-butanol. But the positive values of V^E do not show any regular trends and suggest that the positive V^E values are intensive to the change length of the t-butanol.

The experimental value of ΔK_S may be attributed to the relative strength of effects which influenced the free space (23) according to which positive values of ΔK_S , arise due to breaking of hydrogen bonds in self associated alcohols and physical dipole-dipole interaction between alcohol monomers and multimers contribute to increase in free space, decrease in sound velocity and positive deviation in isentropic compressibility. However, this effect will be counteracted by change of free volume in real mixture and the presence of π -electron in xylene molecules resulting in the formation of OH----- π electron Hydrogen-bonded complexes.

IR measurement for mixture of t-butanol with xylenes over the entire composition range has been carried out in Table-5.

The change in frequencies values of -OH.

IR frequencies of -OH group is calculated as

$\Delta\nu$ = IR frequencies of -OH group of mixture - IR frequencies of -OH group in the pure t-butanol

It is seen that the $\Delta\nu$ values are negative for xylenes, it is concluded that there is a variable degree of intermolecular H-bonding between the components of mixtures.

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Table 1. Mole fraction of xylenes (X_1) and Excess volume (V^E) for the mixture of o-xylene, m-xylene and p-xylene with t-butanol at 303.15 J

t-butanol +	X_1	V^E
o-xylene	0.0000	0.000
	0.1003	0.169
	0.2009	0.283
	0.3016	0.383
	0.3990	0.427
	0.4999	0.451
	0.5998	0.426
	0.6988	0.390
	0.7997	0.287
	0.9003	0.180
	1.0000	0.000

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m-xylene	0.0000	0.000
	0.0957	0.219
	0.1947	0.375
	0.2956	0.490
	0.4002	0.570
	0.5001	0.600
	0.6001	0.560
	0.7003	0.487
	0.7994	0.381
	0.8995	0.200
	1.0000	0.000
p-xylene	0.0000	0.000
	0.0994	0.212
	0.1972	0.362
	0.2992	0.467
	0.4004	0.527
	0.4976	0.548
	0.6002	0.514
	0.6968	0.448
	0.7993	0.350
	0.8980	0.195
	1.0000	0.000

Table2. Standard deviation and values of constant from the Redlich-Kister equation

System t-Butanol +	a_0	a_1	a_2	σ
o-xylene	1.7747	0.0566	0.2051	0.0076
m-xylene	2.3604	-0.1178	0.0187	0.0082
p-xylene	2.1694	-0.1275	0.1313	0.0037

Table3. Mole fraction (X_1) density (ρ) sound velocity (u) isentropic compressibility (K_S) and deviation in isentropic compressibility (ΔK_S) of t-butanol + xylenes at 303.15 K.

t-butanol +	x_1	$\rho \times 10^{-3}$ kg m ⁻³	u m s ⁻¹	K_S TPa ⁻¹	ΔK_S TPa ⁻¹
o-xylene	0.0000	0.8716	1333	646	0
	0.1003	0.8626	1304	682	4
	0.2009	0.8536	1277	719	7
	0.3016	0.8443	1251	757	10
	0.3990	0.8353	1226	796	12
	0.4999	0.8257	1203	836	13
	0.5998	0.8161	1182	878	14
	0.6988	0.8062	1162	919	13
	0.7997	0.7961	1143	962	11
	0.9003	0.7855	1125	1005	6
	1.0000	0.7750	1109	1049	0
m-xylene	0.0000	0.8555	1301	691	0
	0.0957	0.8479	1277	724	6
	0.1947	0.8402	1253	758	11
	0.2956	0.8323	1231	793	15
	0.4002	0.8240	1209	830	18
	0.5001	0.8160	1190	866	19
	0.6001	0.8081	1171	903	20
	0.7003	0.8000	1154	939	18
	0.7994	0.7918	1138	976	14
	0.8995	0.7836	1123	1012	8
	1.0000	0.7750	1109	1049	0
p-xylene	0.0000	0.8522	1294	701	0
	0.0994	0.8447	1271	732	4
	0.1972	0.8374	1250	764	8

	0.2992	0.8298	1228	799	12
	0.4004	0.8222	1208	833	14
	0.4976	0.8148	1190	867	16
	0.6002	0.8070	1171	904	17
	0.6968	0.7995	1154	939	16
	0.7993	0.7913	1138	976	13
	0.8980	0.7834	1123	1012	8
	1.0000	0.7750	1109	1049	0

Table4. Experimental and predicted velocity data for the binary mixture of *t*-butanol + xylenes at 303.15 K

t-butanol +	x_1	Ultrasonic Velocity m.s^{-1}		
		Expt.	CFT	FLT
o-xylene	0.0000	1333	1333	969
	0.1003	1304	1312	975
	0.2009	1277	1291	982
	0.3016	1251	1270	991
	0.3990	1226	1249	1002
	0.4999	1203	1227	1014
	0.5998	1182	1205	1029
	0.6988	1162	1182	1045
	0.7997	1143	1158	1065
	0.9003	1125	1133	1086
	1.0000	1109	1109	1112
m-xylene	0.0000	1301	1301	972
	0.0957	1277	1284	975
	0.1947	1253	1266	981
	0.2956	1231	1248	989
	0.4002	1209	1229	999
	0.5001	1190	1210	1011
	0.6001	1171	1191	1025
	0.7003	1154	1171	1042
	0.7994	1138	1151	1062
	0.8995	1123	1130	1085
	1.0000	1109	1109	1112
p-xylene	0.0000	1294	1294	972
	0.0994	1271	1278	977
	0.1972	1250	1261	983
	0.2992	1228	1243	991
	0.4004	1208	1225	1001
	0.4976	1190	1208	1012
	0.6002	1171	1189	1027
	0.6968	1154	1170	1043
	0.7993	1138	1150	1063
	0.8980	1123	1130	1085
	1.0000	1109	1109	1112

Table5. IR Frequencies ($\nu \text{ cm}^{-1}$) for *t*-Butanol with Xylenes

Mole fraction of t-Butanol	ν (O-H)
o-Xylene	-
0.2	3362.04
0.4	3367.82
0.5	3362.04
0.6	3348.54
0.8	3329.25
t-Butanol	3377.47

m-Xylene

Mole fraction of t-Butanol	ν (O-H)
m-Xylene	-
0.2	3379.75

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0.4	3358.18
0.5	3350.48
0.6	3346.61
0.8	3342.88
t-Butanol	3377.47

p-Xylene

Mole fraction of t-Butanol	ν (O-H)
p-Xylene	-
0.2	3373.61
0.4	3373.61
0.5	3367.82
0.6	3369.75
0.8	3331.18
t-Butanol	3377.47

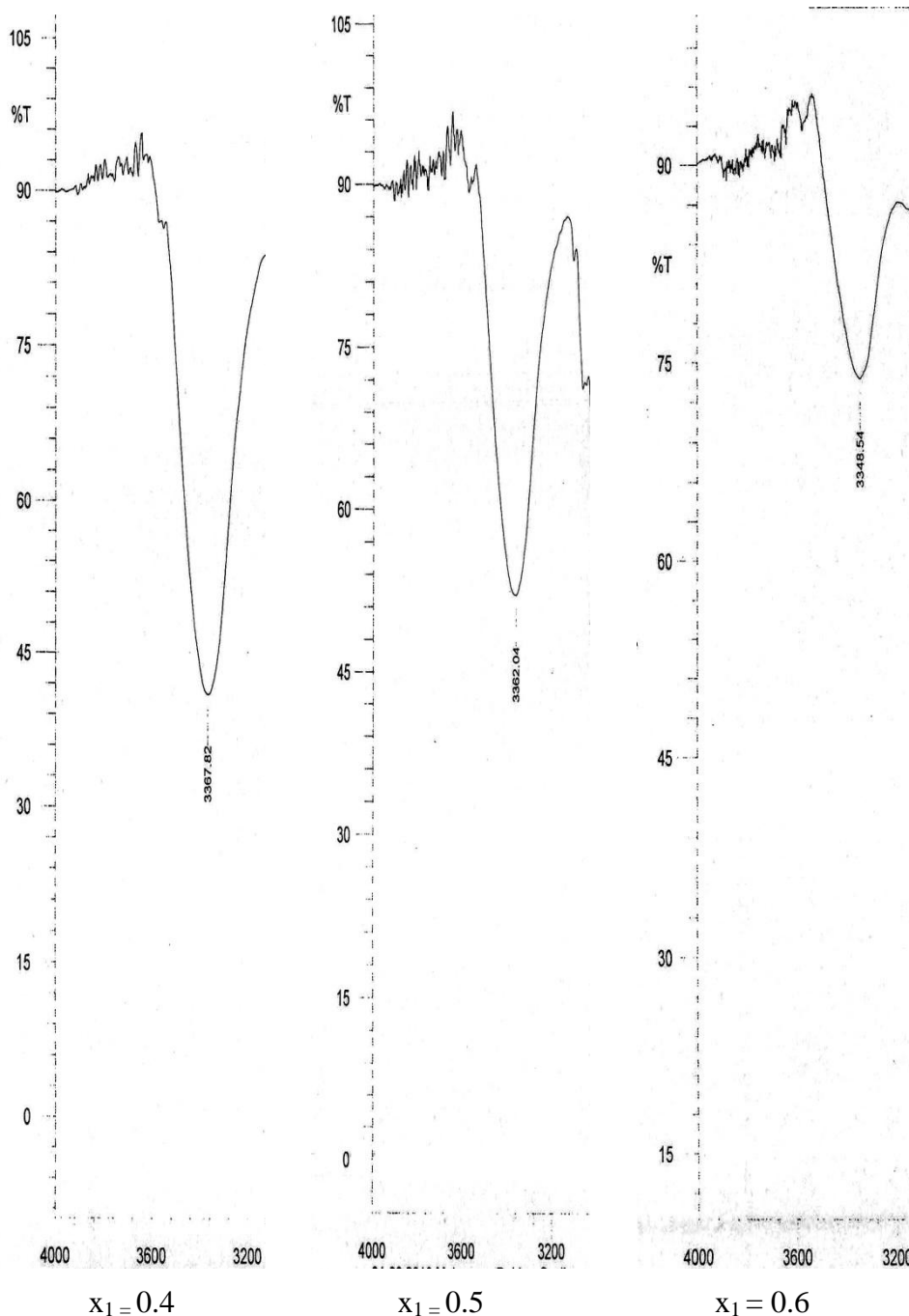


Figure1. Neat FTIR -OH Frequency (cm^{-1}) Cut Section (Spectrum) of t-Butanol + o-Xylene

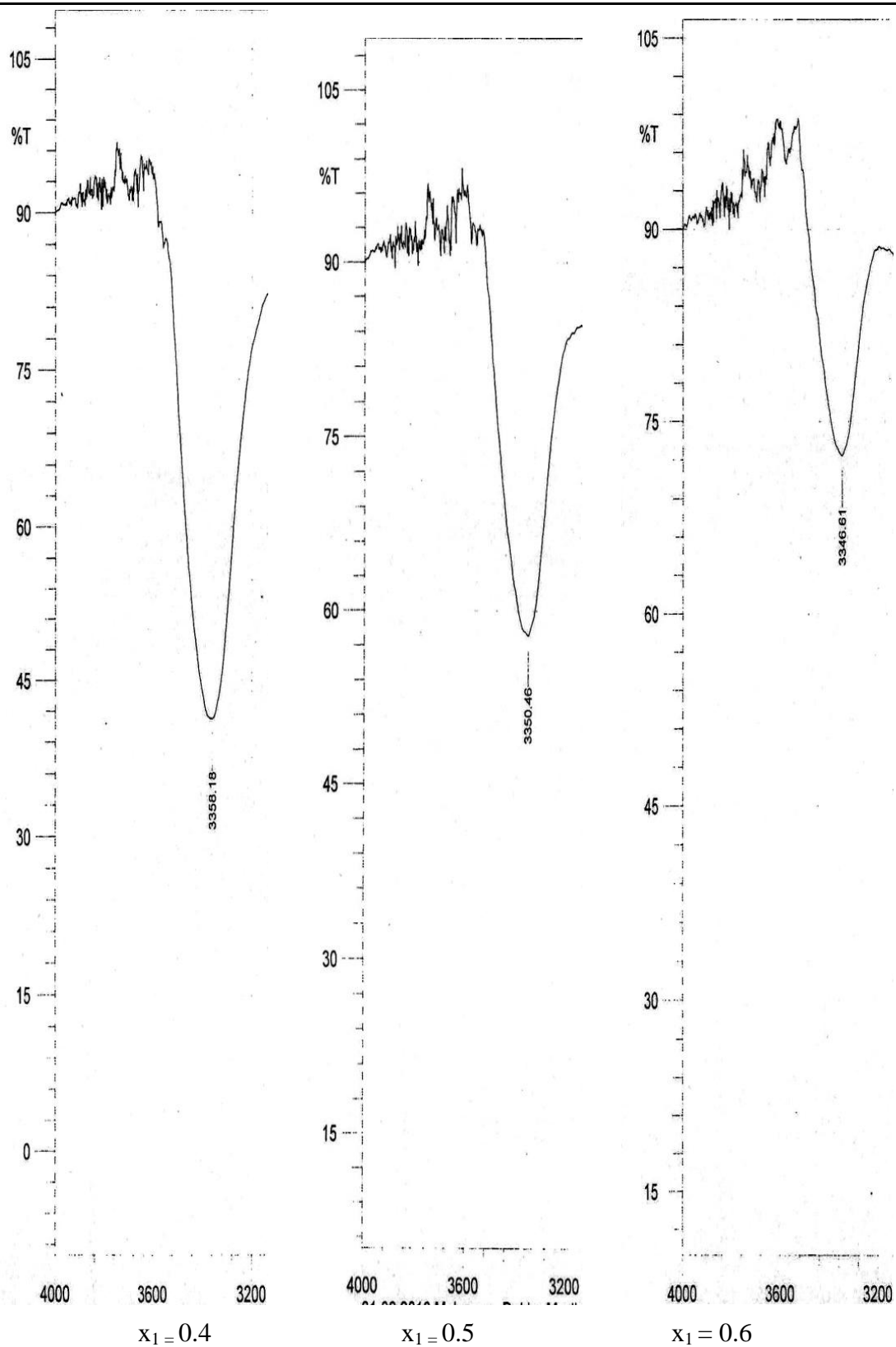


Figure2. Neat FTIR -OH Frequency (cm^{-1}) Cut Section (Spectrum) of *t*-Butanol + *m*-Xylene.

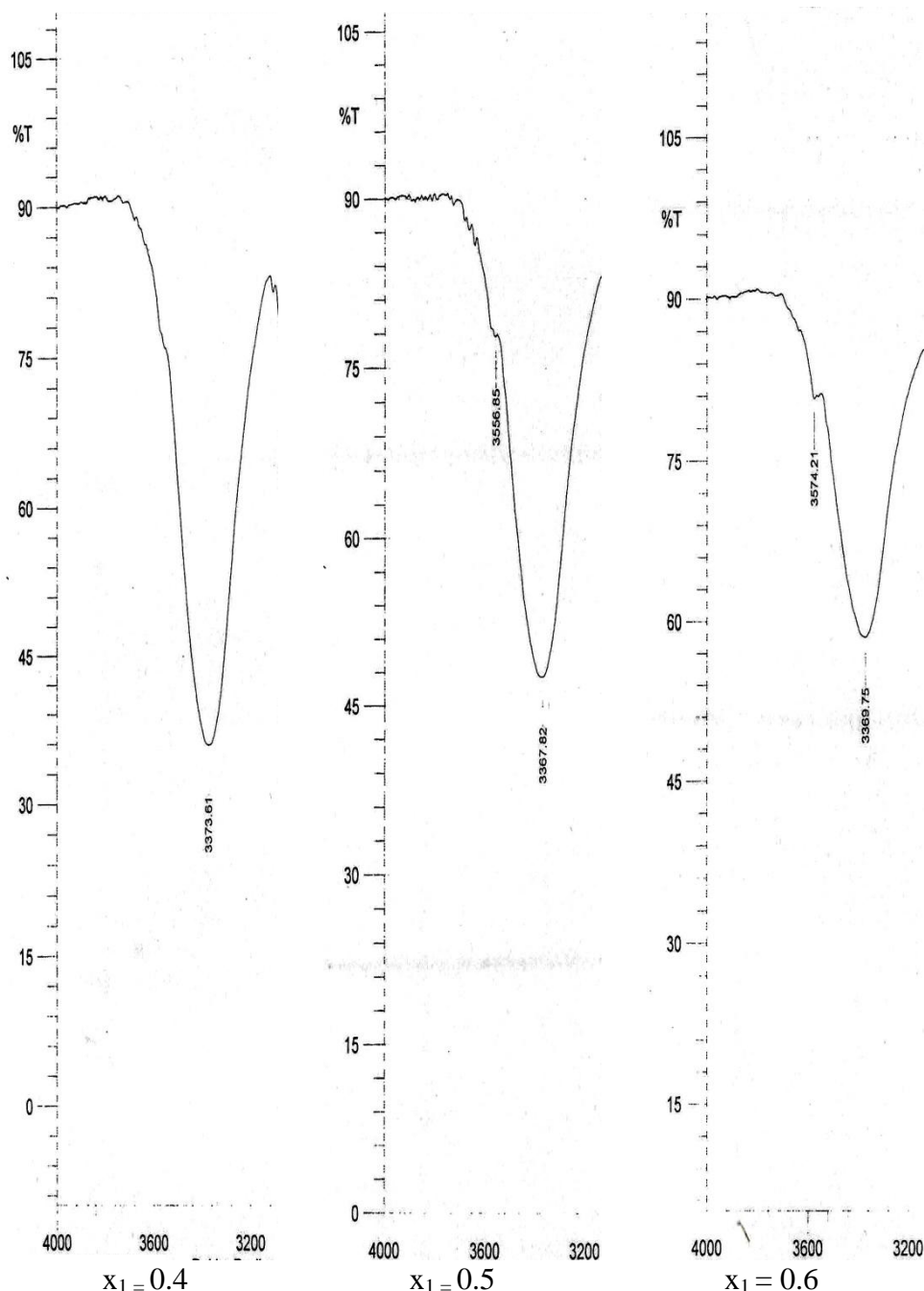


Figure3. Neat FTIR -OH Frequency (cm^{-1}) Cut Section (Spectrum) of *t*-Butanol + *p*-Xylene

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