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BEHAVIOUR OF BENZONITRILE IN THE BINARY MIXTURE OF 2-BUTOXY ETHANOL + N-PROPANOL-AN ULTRASONIC INVESTIGATION

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ABSTRACT

Ultrasonic velocity, density and viscosity measurements have been made experimentally first in the binary mixture- 2 butoxy ethanol + 1 propanol and then in the ternary mixture with benzonitrile as the third component at three temperatures 30, 40 and 50^{o}C. Thermodynamic and other allied parameters (β, π, H, G etc.,) and their excess values have been computed and the intermolecular interactions are estimated in the light of these excess parameters. Weak intermolecular interactions and dispersion forces dominate in the binary system. Addition of benzonitrile to the binary (2 buotoxy ethanol+ n propanol at different concentrations of 2butoxy ethanol) brings about strong intermolecular interactions besides dipole – dipole interactions in the mixed ternary system. In the first ternary (low benzonitrile concentration) endothermic interactions observed at 30^{o}C, transform into exothermic at 50^{o}C. In the other ternaries, exothermic are noticed at all temperatures. Almost all the theories applied to evaluate velocities theoretically agree with the experiment.

Key words: Ultrasonic velocity, ternary mixtures, adiabatic compressibility, inter molecular interactions.

1. INTRODUCTION

Though several ternary mixtures have been studied extensively, ternary mixtures of the binary system of alcohols + alkoxy alcohols with a third component are not studied systematically in the direction of ultrasonic propagation in the total system. Though it is a ternary mixture in essence studied, it will be appropriate to call the study as study of the behaviour of the third component in the binary system of alcohols + alkoxy alcohols. Several ternary mixtures containing one of the components as alkanols/alkoxy alkanols have been ultrasonically studied (Dominquez M et al. 2000; Salas JA et al. 2006; Thirumaran S and Deepesh George, 2009; Thirumaran S and Earnest Jayakumar J, 2009; Thirumaran S and Thenmozhi , 2010; Thirumaran S and Sudha S, 2010; Sumathi T and Abeetha K, 2011) in the direction of theoretical evaluation of velocities and intermolecular associations/interactions in the whole system. Glory J et al. 2009; have studied the behaviour of nitrobenzene in the binary system, n-butanol + 2-methoxy ethanol at three concentrations at 30^{o}C. The study of the three chemical compounds chosen in the present investigation has been taken up owing to their application / use in chemistry / medicine. Benzonitrile is a very good solvent besides being used in forming co-ordinate complexes. 2 butoxy ethanol is a solvent in paints, surface coatings, glass cleaners as well as domestic commercial cleaning solutions (as a main ingradient). n-propanol is a solvent in pharmaceutical industry and used in cellulose esters and fermentation process. In the

present investigation, an attempt is made to study the behaviour of benzonitrile in the binary mixture of n-propanol + 2 butoxy ethanol at three temperatures. At first the binary system has been studied at various concentrations of 2 butoxy ethanol by measuring ultrasonic velocity, density and viscosity at three temperatures 30, 40 & 50^{o}C and then by adding the third component i.e. benzonitrile to the binary system at various concentrations, the above measurements have been repeated. The molecular interactions in the binary system and the effect of the third component on the binary system at different concentrations of benzonitrile in the system have been estimated using the excess thermodynamic parameters computed. Mostly strong AB interactions (between the constituent unlike molecules) have been suggested in both the binary and ternary systems. Also it has been observed that the degree of interaction has become strengthened with the addition of benzonitrile at all temperatures studied. Mostly exothermic interactions have been indicated at 30^{o}C and endothermic at 40 and 50^{o}C.

2. EXPERIMENTAL

Ultrasonic velocity is measured employing a single crystal variable path ultrasonic interferometer working at 2MHz (Mittal Enterprises, New Delhi) with an accuracy of ± 0.05 %. Density is measured using a double stem capillary type pyknometer with an accuracy of 2 parts in 10^5. Ostwald Viscometer is employed in viscosity determination, the uncertainty being ± 0.1 %. Temperature stability to within ± 0.01 K is maintained in the constant temperature water bath. For standardization of velocity, triple distilled water is used as a reference liquid. All the details are presented elsewhere (Yanadi Reddy N et al. 2004; Jayamadhuri N et al. 2011) . All the chemicals used are of analar grade/sd fine and are further purified by using the standard methods (Furniss AS et al. 1980) .

3. THEORETICAL

Using the following standard formulae, various thermodynamic and other related parameters are computed.

Adibatic compressibility $$\beta = \frac{1}{U_{exp}^2 \rho_{exp}} \quad \text{---- (1)}$$

Internal pressure $$\pi = bRT\left[\frac{K\eta}{U}\right]^{1/2} \frac{\rho^{2/3}}{M^{7/6}} \quad \text{---- (2)}$$

Enthalpy $$H = \pi V_M \quad \text{---- (3)}$$

Gibb's activation energy $$G = RT[\ln \eta V_M] \quad \text{---- (4)}$$

Seven theories – FLT due to Jacobson, CFT due to Schaaffs, NOMOTO, VANDAEL and JUNJIE, KT, J-A theories have been employed to evaluate the ultrasonic velocities theoretically in the mixture. All the details regarding the above equations and theories are dealt with elsewhere (Yanadi Reddy N et al. 2004; Naidu et al. 2012).

4. RESULTS AND DISCUSSION

Ultrasonic velocity, density and viscosity have been measured in the binary mixture: 2-butoxy ethanol + n-propanol as a function of the concentration of butoxy ethanol at three temperatures 30, 40 and 50^{o}C. In order to study the behaviour of another component (nitro component), benzonitrile in the binary mixture, velocity, density and viscosity measurements have also been made at various concentrations of benzonitrile (the third component) in the said binary mixture.

As seen earlier in our previous paper, in the binary mixture 2 propanol+ 2 butoxy ethanol, almost all theories agree well with the experiment in evaluating velocities theoretically in general and KT and JA in particular (with more accuracy). From the

computed thermodynamic and other allied parameters and their excess values, it may be said that inter molecular interactions are weak between the two constituents besides dispersive forces dominating at 30^{o}C. Endothermic type of chemical reactions are suggested and all these interactions become weaker as the temperature is increases from 30 to 50^{o}C.

It is of interest to study the effect of the third component, benzonitrile on the binary mixture at various concentrations. Here 'butoxy ethanol + propanol' is taken as co solvent for the third component, benzonitrile and seven such ternaries are studied as follows.

1. Benzonitrile +A (2butoxy ethanol+ n propanol at 0.1760 mole fraction of 2 butoxyethanol)
2. Benzonitrile +B (2butoxy ethanol+ n propanol at 0.2456 mole fraction of 2 butoxyethanol)
3. Benzonitrile +C (2butoxy ethanol+ n propanol at 0.3219 mole fraction of 2 butoxyethanol)
4. Benzonitrile +D (2butoxy ethanol+ n propanol at 0.4061 mole fraction of 2 butoxyethanol)
5. Benzonitrile +E (2butoxy ethanol+ n propanol at 0.5000 mole fraction of 2 butoxyethanol)
6. Benzonitrile +F (2butoxy ethanol+ n propanol at 0.6031 mole fraction of 2 butoxyethanol)
7. Benzonitrile +G (2butoxy ethanol+ n propanol at 0.7219 mole fraction of 2 butoxyethanol)

Ultrasonic velocity, density and viscosity have been measured in all the above seven ternaries at 30, 40 and 50^{o}C over the entire composition range of benzonitrile and are presented in Tables 1.1-1.7. As observed from tables, velocity increases with the concentration of benzonitrile at all temperatures and decrease of velocity increases with the concentration of benzonitrile at all temperatures and decrease of velocity with rise in temperature is noticed. Though the increase in velocity is nonlinear, on the whole, mostly linear increase is observed from the first concentration i.e., from 0.05 m of benzonitrile. From a comparison of the theoretical velocities with experimental ones as shown in Figs. 1.1 – 1.7, it may be seen that except in the ternary system with F, the deviations are not large and almost all the theories appear to agree well with the experiment. From the thermo dynamical and other related parameters computed (Table 2.1 – 2.3) given for systems with A, E and G i.e A rich, equimolar and benzonitrile rich concentrations), it is seen that in all the three ternaries, adiabatic compressibility (β), free length (L_f), internal pressure (π), enthalpy (H) and Gibb's activation energy (G) all decrease with concentration at all temperatures while β, L_f and V_m increase with temperature at all concentrations. Now to assess the nature of chemical interactions and intermolecular interactions between benzonitrile and the binary (A, E or G, in the mixed system), the excess parameters have been calculated and presented in Figs.2.1 – 2.3. As seen from the figures, the behaviour of β^E is the same in the system with A and E where as it is negative throughout with a minimum at ~0.15m and less negative at 50^{o}C in the system with G. L_f^E is similar to β^E. π^E is positive at low concentrations (upto 0.2m) and thereafter negative at high concentrations at all temperatures and is more negative at 50^{o}C in the system with A. In other system i.e, with E and G, it is totally negative. H^E is similar to π^E at all temperatures- more negative at 50^{o}C except in G system. G^E is totally positive at 30^{o}C, positive up to ~0.6m at 40^{o}C and negative throughout at 50^{o}C in the first ternary (with A). Negative throughout and more negative at 50^{o}C in the E system while in the last ternary (with G), less negative at 50^{o}C. More or less similar behaviour is observed in η^E in all the systems.

Table 1.1. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + A (2 butoxy ethanol + n propanol 0.1760 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
30^0C			
0.0000	1178.1	819.39	1.60978
0.0498	1304.0	905.95	1.81256
0.0999	1314.6	912.38	1.75219
0.2985	1324.6	920.89	1.66393
0.4982	1340.4	935.83	1.53837
0.5983	1348.8	944.10	1.43904
0.6985	1361.6	955.18	1.35578
0.8993	1385.4	976.73	1.11888
0.9497	1392.9	985.15	1.06414
1.0000	1402.5	995.00	1.10441
40^0C			
0.0000	1167.7	809.96	1.25900
0.0498	1276.2	881.25	1.42356
0.0999	1287.7	890.84	1.36582
0.2985	1309.0	911.16	1.25074
0.4982	1332.2	927.65	1.12645
0.5983	1342.8	936.31	1.06478
0.6985	1350.0	946.15	0.99728
0.8993	1366.6	970.61	0.91542
0.9497	1372.2	979.04	0.90226
1.0000	1376.4	988.47	0.97315
50^0C			
0.0000	1162.6	804.70	1.18829
0.0498	1242.6	869.83	1.17802
0.0999	1245.3	872.15	1.15239
0.2985	1248.1	880.42	1.07253
0.4982	1259.9	898.35	0.97327
0.5983	1264.4	908.84	0.94091
0.6985	1273.2	918.94	0.92068
0.8993	1288.2	953.39	0.85175
0.9497	1313.0	965.97	0.83009
1.0000	1327.2	977.07	0.89534

Table 1.2. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + B (2 butoxy ethanol + n propanol 0.2456 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
30^0C			
0.0000	1187.2	823.58	1.67138
0.0999	1282.6	873.33	1.44533
0.2985	1312.8	892.08	1.37914
0.4982	1343.6	922.81	1.25040
0.5983	1356.9	935.70	1.16634
0.6985	1368.2	953.49	1.12418
0.8993	1388.0	977.92	1.07178
1.0000	1402.5	995.00	1.10441
40^0C			
0.0000	1180.0	818.93	1.31362
0.0999	1262.1	880.20	1.26082
0.2985	1293.7	899.63	1.12002
0.4982	1315.0	923.44	0.96591
0.5983	1325.4	935.70	0.91514
0.6985	1335.0	946.16	0.86899
0.8993	1364.5	972.92	0.80486
1.0000	1376.4	988.47	0.97315
50^0C			
0.0000	1173.9	812.10	1.26877
0.0999	1233.6	834.08	1.10771
0.2985	1258.9	854.92	0.96584
0.4982	1280.4	898.48	0.86825
0.5983	1293.0	915.67	0.82779
0.6985	1304.4	932.86	0.81478
0.8993	1320.8	959.24	0.79275
1.0000	1327.2	977.07	0.89534

Table 1.3. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + C (2 butoxy ethanol + n propanol 0.3129 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
30^0C			
0.0000	1206.2	834.88	1.73639
0.0999	1291.2	865.47	1.57245
0.2985	1321.2	893.70	1.44146
0.4982	1341.6	923.24	1.22323
0.5983	1352.3	935.70	1.11230
0.6985	1366.8	946.85	0.94787
0.8993	1382.4	974.76	0.92289
1.0000	1402.5	995.00	1.10441
40^0C			
0.0000	1192.6	826.89	1.36601
0.0999	1246.0	853.63	1.21969
0.2985	1269.6	884.86	0.99222
0.4982	1291.0	911.71	0.87163
0.5983	1304.5	926.53	0.83514
0.6985	1315.6	941.10	0.79645
0.8993	1342.8	968.56	0.75922
1.0000	1376.4	988.47	0.97315
50^0C			
0.0000	1187.5	819.77	1.32913
0.0999	1228.2	847.72	1.12648
0.2985	1254.8	882.54	0.89472
0.4982	1279.2	908.84	0.83256
0.5983	1288.5	923.50	0.83009
0.6985	1299.0	930.98	0.78340
0.8993	1317.2	954.52	0.74263
1.0000	1327.2	977.07	0.89534

Table 1.4. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + D (2 butoxy ethanol + n propanol 0.4061 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
30^0C			
0.0000	1227.1	851.88	1.80547
0.0999	1308.0	891.96	1.79516
0.2985	1332.0	907.91	1.52793
0.4982	1350.0	921.00	1.36492
0.5983	1356.0	933.27	1.25460
0.6985	1377.2	958.93	1.05921
0.8993	1383.6	981.72	1.04243
1.0000	1402.5	995.00	1.10441
40^0C			
0.0000	1223.8	849.91	1.52186
0.0999	1272.0	872.30	1.48696
0.2985	1284.0	902.07	1.18294
0.4982	1292.9	914.55	1.04736
0.5983	1303.2	923.99	0.98495
0.6985	1323.3	948.13	0.89295
0.8993	1350.0	973.35	0.87827
1.0000	1376.4	988.50	0.97315
50^0C			
0.0000	1219.4	842.28	1.43994
0.0999	1243.5	872.53	1.43562
0.2985	1263.0	892.68	1.12045
0.4982	1273.2	900.66	1.04478
0.5983	1281.5	913.56	0.99476
0.6985	1296.0	935.24	0.93537
0.8993	1316.0	962.96	0.88974
1.0000	1327.2	977.07	0.89534

Table 1.5. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + E (2 butoxy ethanol + n propanol 0.5000 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
30^0C			
0.0000	1227.1	851.88	1.80547
0.0999	1294.0	891.35	1.69734
0.2985	1316.5	916.25	1.47997
0.4982	1336.4	934.17	1.29983
0.5983	1346.9	946.31	1.19604
0.6985	1359.6	961.03	1.11748
0.8993	1387.3	986.27	1.03203
1.0000	1402.5	995.00	1.10441
40^0C			
0.0000	1223.8	849.91	1.52186
0.0999	1263.6	890.30	1.37115
0.2985	1290.1	911.36	1.15856
0.4982	1315.2	927.28	0.99960
0.5983	1331.4	939.69	0.91514
0.6985	1344.0	952.63	0.88104
0.8993	1364.7	975.04	0.76718
1.0000	1376.4	988.47	0.97315
50^0C			
0.0000	1219.4	842.28	1.43994
0.0999	1235.8	873.13	1.20171
0.2985	1260.9	900.83	1.07141
0.4982	1282.0	923.83	0.96969
0.5983	1292.5	934.46	0.93479
0.6985	1302.3	945.20	0.89373
0.8993	1320.1	967.46	0.85898
1.0000	1327.2	977.07	0.89534

Table 1.6. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + F (2 butoxy ethanol + n propanol 0.6031 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
30^0C			
0.0000	1242.5	860.75	1.85472
0.0999	1298.0	887.35	1.66733
0.2985	1316.4	901.54	1.52136
0.4982	1339.2	924.73	1.25624
0.5983	1352.0	935.70	1.16322
0.6985	1368.0	949.71	1.12882
0.8993	1393.5	975.77	1.10889
1.0000	1402.5	995.00	1.10441
40^0C			
0.0000	1238.2	857.65	1.56011
0.0999	1263.6	869.13	1.19267
0.2985	1276.1	885.95	1.10566
0.4982	1297.2	916.16	0.93627
0.5983	1311.5	928.63	0.88919
0.6985	1327.5	941.50	0.85683
0.8993	1355.7	972.05	0.78617
1.0000	1376.4	988.47	0.97315
50^0C			
0.0000	1233.3	852.96	1.46997
0.0999	1263.1	866.33	1.23383
0.2985	1272.2	880.57	1.14538
0.4982	1289.1	913.70	0.91514
0.5983	1296.7	927.23	0.87743
0.6985	1306.5	939.86	0.85205
0.8993	1320.0	963.62	0.82105
1.0000	1327.2	977.07	0.89534

Table 1.7. ***Ultrasonic velocity, density and viscosity as a function of concentration of benzonitrile in the mixture: Benzonitrile + G (2 butoxy ethanol + n propanol 0.7219 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Velocity (ms^{-1})	Density ($kg\ m^{-3}$)	Viscosity (milli Pa.s)
	30^0C		
0.0000	1258.5	873.12	1.87062
0.0497	1308.0	905.96	1.68028
0.0999	1316.7	915.05	1.56113
0.2985	1335.0	936.60	1.37859
0.4982	1347.0	954.80	1.22323
0.5983	1358.0	964.40	1.16982
0.6985	1376.0	972.34	1.11888
0.8993	1392.4	985.15	1.08414
0.9497	1398.0	990.25	1.06802
1.0000	1402.5	995.00	1.10441
	40^0C		
0.0000	1251.4	867.75	1.58477
0.0497	1302.2	880.78	1.46413
0.0999	1306.8	887.84	1.40314
0.2985	1323.3	909.07	1.25074
0.4982	1339.3	927.65	1.12645
0.5983	1346.5	938.53	1.07081
0.6985	1355.3	950.35	0.99728
0.8993	1368.6	972.16	0.98318
0.9497	1372.8	979.81	0.97891
1.0000	1376.2	988.47	0.97315
	50^0C		
0.0000	1245.1	864.23	1.49009
0.0497	1248.7	882.62	1.19825
0.0999	1253.6	889.31	1.16573
0.2985	1269.0	912.29	1.07860
0.4982	1282.0	929.06	1.00983
0.5983	1290.9	939.58	0.97124
0.6985	1299.8	950.61	0.93484
0.8993	1318.8	965.95	0.87603
0.9497	1323.3	972.16	0.86591
1.0000	1327.2	977.07	0.89534

Table 2.1. ***Thermodynamic/Acoustical parameters computed in the mixture: Benzonitrile + A (2 butoxy ethanol + n propanol 0.1760 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Adiabatic Compressibility (10^{-10} N^{-1} m^2)	Internal Pressure (atms)	Free Length (A^0)	Molar Volume (10^{-3}L.mole^{-1})	Enthalpy (KJ mole^{-1})	Gibb's Energy (RT units)
			30^0C			
0.0000	8.79	7458	0.59170	76.91	574	4.82
0.0498	6.49	7255	0.50839	71.77	557	4.87
0.0999	6.34	7164	0.50251	73.46	541	4.86
0.2985	6.19	6310	0.49641	81.43	514	4.91
0.4982	5.95	5416	0.48663	88.69	480	4.92
0.5983	5.82	4971	0.48147	92.16	458	4.89
0.6985	5.65	4592	0.47417	95.30	437	4.86
0.8993	5.33	3802	0.46086	101.44	386	4.79
0.9497	5.23	3632	0.45641	102.63	376	4.69
1.0000	5.11	3628	0.45104	103.64	373	4.74
			40^0C			
0.0000	9.05	6574	0.60044	77.81	511	4.58
0.0498	6.97	6320	0.52670	73.78	503	4.65
0.0999	6.77	6165	0.51918	75.24	486	4.63
0.2985	6.41	5465	0.50500	82.30	450	4.63
0.4982	6.07	4622	0.49178	89.47	414	4.61
0.5983	5.92	4262	0.48563	92.93	396	4.59
0.6985	5.80	3930	0.48052	96.21	378	4.56
0.8993	5.52	3448	0.46867	102.08	352	4.54
0.9497	5.42	3356	0.46474	103.27	347	4.53
1.0000	5.34	3423	0.46111	104.32	357	4.62
			50^0C			
0.0000	9.19	6373	0.60504	78.3	499	4.53
0.0498	7.45	6233	0.54448	74.7	466	4.48
0.0999	7.39	5954	0.54257	76.9	458	4.49
0.2985	7.29	5065	0.53881	85.2	431	4.51
0.4982	7.01	4324	0.52841	92.4	399	4.50
0.5983	6.88	4048	0.52348	95.7	388	4.50
0.6985	6.71	3813	0.51700	99.1	378	4.51
0.8993	6.32	3385	0.50166	103.9	352	4.48
0.9497	6.00	3261	0.48897	104.7	341	4.46
1.0000	5.81	3317	0.48098	105.5	350	4.55

Table 2.2. ***Thermodynamic/Acoustical parameters computed in the mixture: Benzonitrile + E (2 butoxy ethanol + n propanol 0.5000 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Adiabatic Compressibility (10^{-10} N^{-1} m^2)	Internal Pressure (atms)	Free Length (A^0)	Molar Volume (10^{-3}L.mole^{-1})	Enthalpy (KJ mole^{-1})	Gibb's Energy (RT units)
			30^0C			
0.0000	7.80	4598	0.55713	118.17	543	5.36
0.0999	6.70	4462	0.51650	113.22	505	5.26
0.2985	6.30	4184	0.50073	110.67	463	5.10
0.4982	5.99	3920	0.48852	109.07	428	4.95
0.5983	5.82	3768	0.48159	107.93	407	4.86
0.6985	5.63	3652	0.47342	106.53	389	4.78
0.8993	5.27	3515	0.45800	104.31	377	4.68
1.0000	5.11	3628	0.45104	103.64	376	4.74
			40^0C			
0.0000	7.86	4221	0.55928	118.45	499	5.19
0.0999	7.03	4055	0.52924	113.35	460	5.05
0.2985	6.59	3726	0.51234	111.26	415	4.86
0.4982	6.23	3448	0.49823	109.88	379	4.70
0.5983	6.00	3299	0.48891	108.69	358	4.60
0.6985	5.81	3242	0.48103	107.47	348	4.55
0.8993	5.51	3033	0.46825	105.51	340	4.49
1.0000	5.34	3423	0.46111	104.32	357	4.62
			50^0C			
0.0000	7.98	4089	0.56384	119.52	489	5.15
0.0999	7.50	3790	0.54644	115.58	438	4.93
0.2985	6.98	3597	0.52726	112.56	405	4.79
0.4982	6.59	3432	0.51209	110.29	378	4.67
0.5983	6.41	3372	0.50503	109.30	369	4.63
0.6985	6.24	3300	0.49838	108.32	357	4.57
0.8993	5.93	3283	0.48597	106.33	353	4.56
1.0000	5.81	3317	0.48098	105.54	350	4.55

Table 2.3. ***Thermodynamic/Acoustical parameters computed in the mixture: Benzonitrile + G (2 butoxy ethanol + n propanol 0.7219 mole fraction of 2 butoxy ethanol)***

Mole fraction of benzonitrile	Adiabatic Compressibility (10^{-10} N^{-1} m^2)	Internal Pressure (atms)	Free Length (A^0)	Molar Volume (10^{-3}L.mole^{-1})	Enthalpy (KJ mole^{-1})	Gibb's Energy (RT units)
			30^0C			
0.0000	7.23	4014	0.53659	131.96	529	5.51
0.0497	6.45	3848	0.50684	126.52	486	5.36
0.0999	6.30	3744	0.50098	124.60	467	5.27
0.2985	5.99	3638	0.48839	119.16	434	5.10
0.4982	5.77	3545	0.47941	114.36	405	4.94
0.5983	5.62	3538	0.47315	111.97	394	4.88
0.6985	5.43	3535	0.46505	109.81	383	4.81
0.8993	5.24	3522	0.45658	105.91	374	4.74
0.9497	5.17	3486	0.45358	104.75	371	4.72
1.0000	5.11	3628	0.45104	103.64	376	4.74
			40^0C			
0.0000	7.36	3690	0.46118	132.78	489	5.35
0.0497	6.70	3533	0.46436	130.13	460	5.25
0.0999	6.60	3492	0.46761	128.41	448	5.19
0.2985	6.28	3412	0.47759	122.77	419	5.03
0.4982	6.01	3347	0.48373	117.71	394	4.89
0.5983	5.88	3323	0.48917	115.05	382	4.81
0.6985	5.73	3266	0.50012	112.35	367	4.72
0.8993	5.49	3365	0.51245	107.33	361	4.66
0.9497	5.42	3394	0.51632	105.87	359	4.64
1.0000	5.34	3423	0.54130	104.32	357	4.62
			50^0C			
0.0000	7.46	3577	0.54514	133.32	477	5.29
0.0497	7.27	3268	0.53788	129.86	424	5.05
0.0999	7.16	3254	0.53376	128.20	418	5.01
0.2985	6.81	3244	0.52060	122.34	397	4.88
0.4982	6.55	3242	0.51065	117.53	381	4.78
0.5983	6.39	3235	0.50428	114.92	372	4.72
0.6985	6.23	3229	0.49791	112.32	363	4.65
0.8993	5.95	3222	0.48683	108.02	348	4.55
0.9497	5.87	3234	0.48362	106.70	345	4.53
1.0000	5.81	3317	0.48098	105.54	350	4.55

From the behaviour of π^E and H^E at low concentrations, weak interactions and at high concentrations, strong AB interactions are noticed at 30^oC which become stronger further at 50^oC in the first ternary (with A). In the other two systems (with E and G) at all temperatures, strong inter molecular interactions between benzonitrile and the binaries besides dipole – dipole interactions are predicted. At 50^oC interactions become stronger. In the system with A, endothermic interactions observed at 30^oC transfer into exothermic at 50^oC. In the other two systems, exothermic interactions all temperatures are noticed. In the other ternaries (with B,

C, D & F) also, similar behaviour of the excess parameters is noticed and the reactions are also similar.

Also an attempt has been made to calculate the relaxation parameters like relaxation strength, relaxation time and absorption coefficient which are shown in Figs 3-5 for the system with A, E and G. All the three decrease with concentration as well as temperature. Mostly similar type of intermolecular interactions from excess parameters are suggested even from the variation of these parameters.

At this juncture, it is appropriate to compare our results and findings with those of other workers. Our results are in conformity with those of other workers (Salas JA et al. 2006; Thirumaran S and Deepesh George, 2009; Thirumaran S and Thenmozhi, 2010; Sumathi T and Abeetha K, 2011) in other ternary mixtures with either alkanol or alkoxy alkanol as one of the components. Here a mention may also be made to the work of (Glory J et al. 2009) who have worked in the ternary system consisting of n butanol, 2 methoxy ethanol and nitrobenzene. Strong AB interactions have been reported besides dipole-dipole interactions between the co solvent (n butanol + 2 methoxy ethanol) and nitrobenzene. Exothermic nature of chemical reaction is also suggested in the system. (Meenakshi G et al. 2009; Sudharani N and Palaniappan L, 2005; Arul G and Palaniappan L, 2005; Shukla BP et al. 1992; Rama Rao G et al. 2004; Ali A et al. 2004; and Sravana Kumar D et al. 2007) suggested the nature of molecular interactions from the variation of excess parameters in the ternary mixtures with at least one component as alkanol or alkoxy alkanol. From the negative values of majority of the excess parameters, in the present system also similar types of reactions are suggested.

5. CONCLUSIONS

Mostly strong interactions are indicated in the binary mixture as well as the ternary system of the present investigation. Addition of benzonitrile has further strengthened the molecular interactions already existing between the components of the binary system: 2 butoxy ethanol + 1 propanol. The nature of chemical interactions is exothermic at all temperatures.

6. ACKNOWLEDGEMENTS

The authors are thankful to the authorities of SVU PG Centre, Kavali for the facilities provided. One of the authors (JG) is thankful to the UGC for the award of RGNF (SRF).

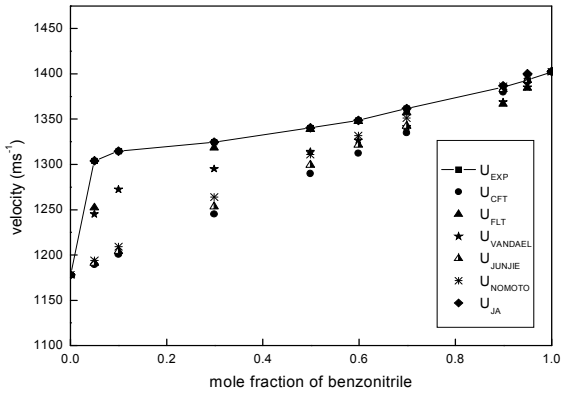

Fig. 1.1 (a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + A (0.1760)

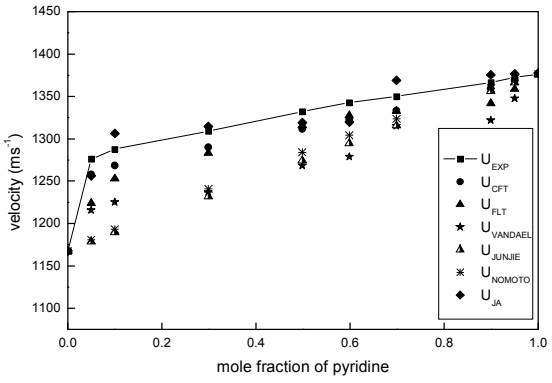

Fig. 1.1 (b). Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + A (0.1760)

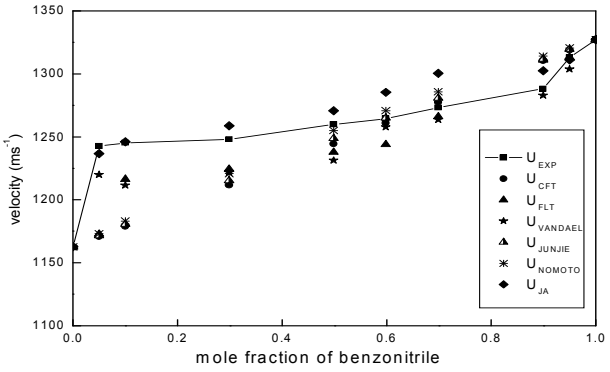

Fig. 1.1 (c). Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + A (0.1760)

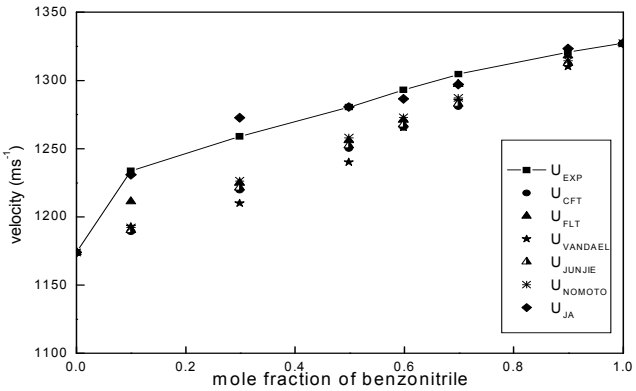

Fig. 1.2 (c). Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + B (0.2456)

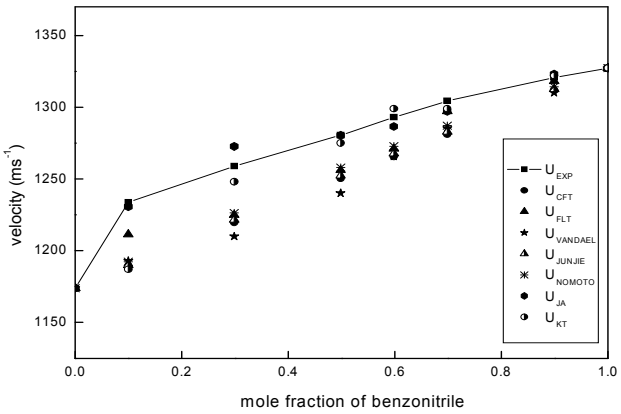

Fig. 1.2 (a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + B (0.2456)

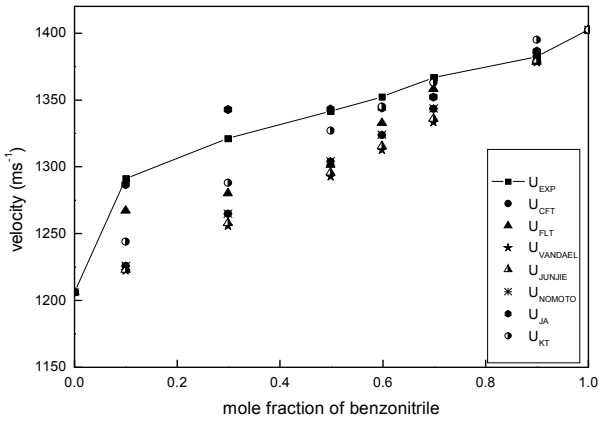

Fig. 1.3 (a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + C (0.3219)

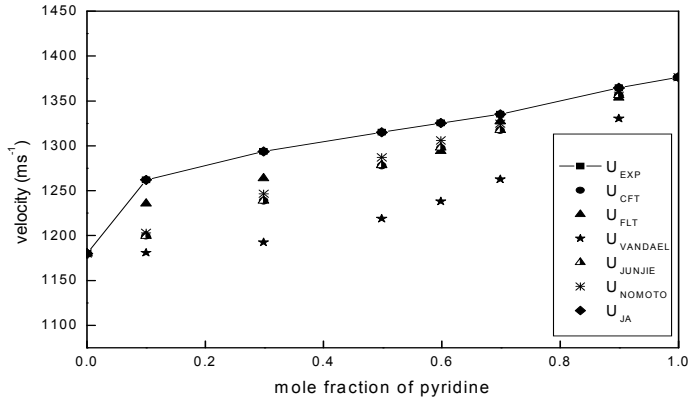

Fig. 1.2 (b). Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + B (0.2456)

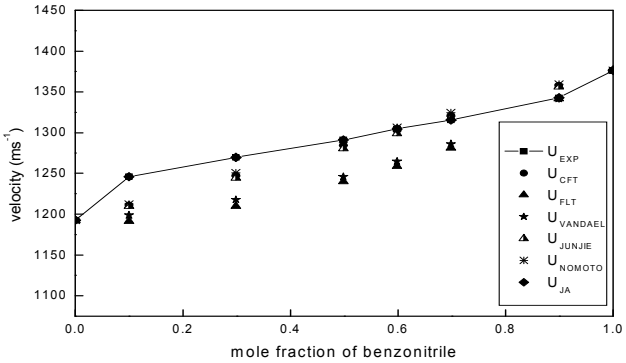

Fig. 1.3 (b).Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + C (0.3219)

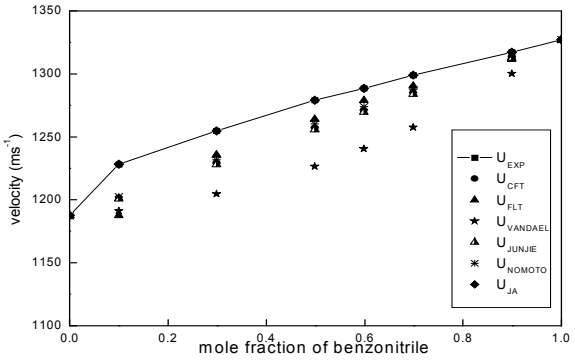

Fig. 1.3 (c).Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + C (0.3219)

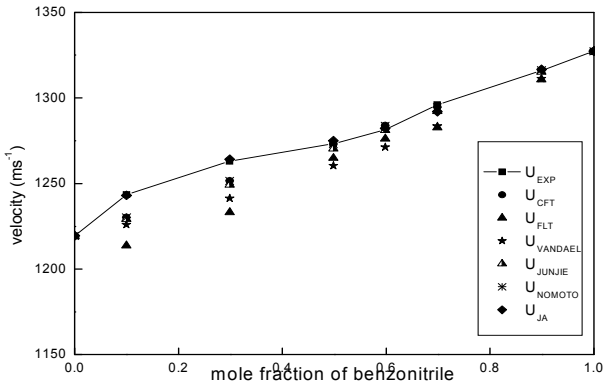

Fig. 1.4 (c). Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + D (0.4061)

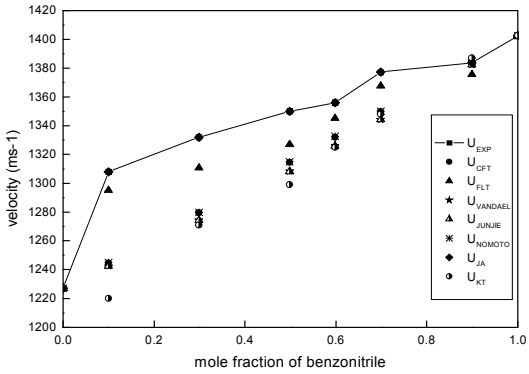

Fig. 1.4 (a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + D (0.4061)

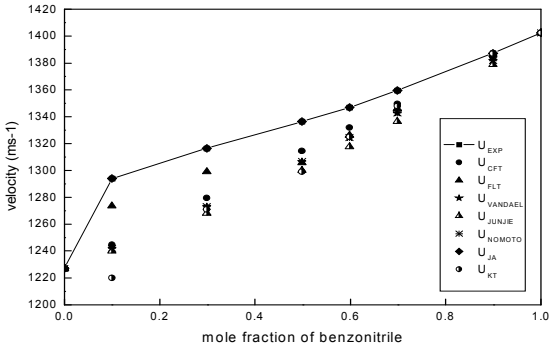

Fig. 1.5(a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + E (0.5000)

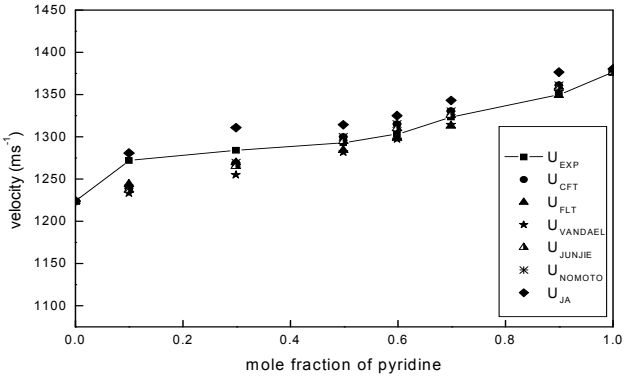

Fig. 1.4 (b). Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + D (0.4061)

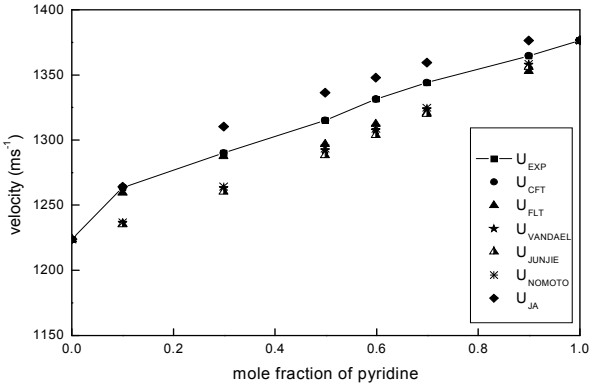

Fig. 1.5(b). Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + E (0.5000)

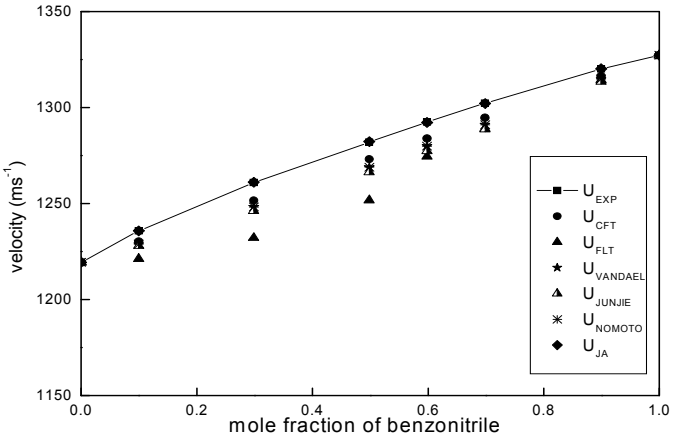

Fig. 1.5 (c).Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + E (0.5000)

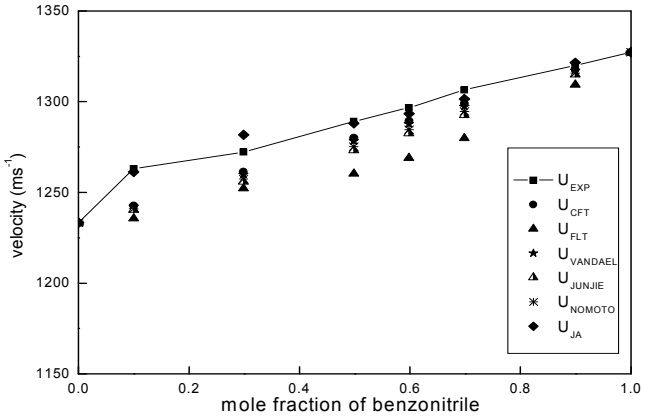

Fig. 1.6 (c). Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + F (0.6031)

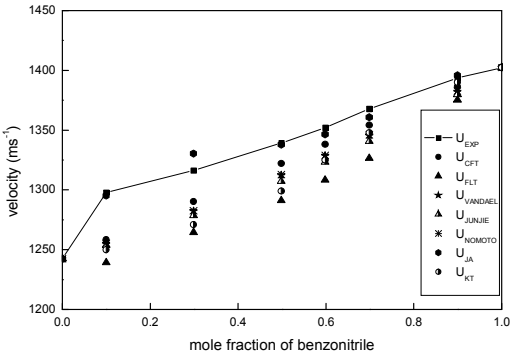

Fig. 1.6 (a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + F (0.6031)

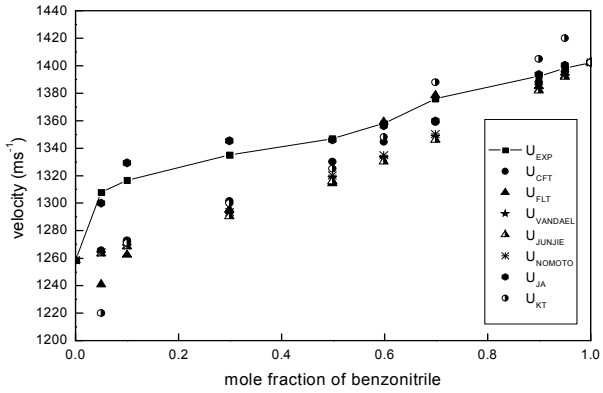

Fig.1.7 (a). Variation of ultrasonic velocity with mole fraction of benzonitrile at 30^{0}C in the mixture: Benzonitrile + G (0.7219)

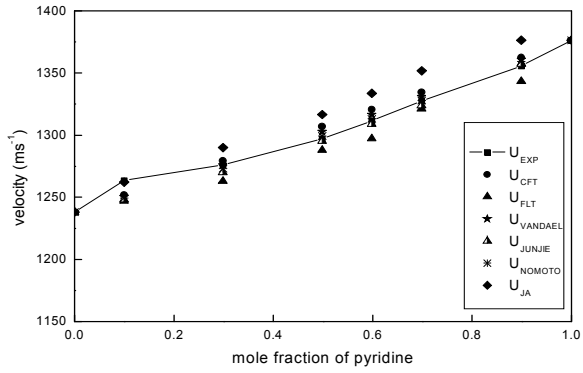

Fig. 1.6 (b). Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + F (0.6031)

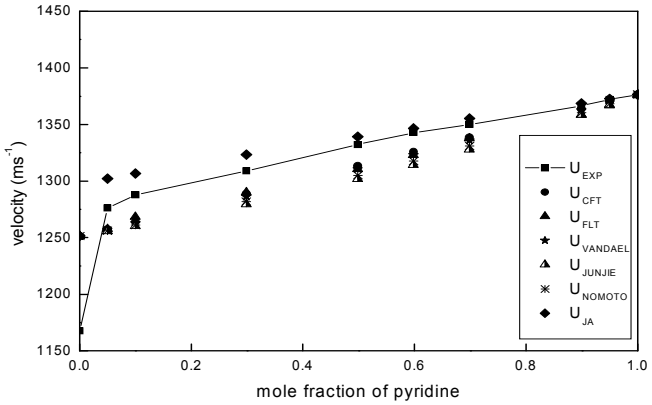

Fig. 1.7 (b). Variation of ultrasonic velocity with mole fraction of benzonitrile at 40^{0}C in the mixture: Benzonitrile + G (0.7219)

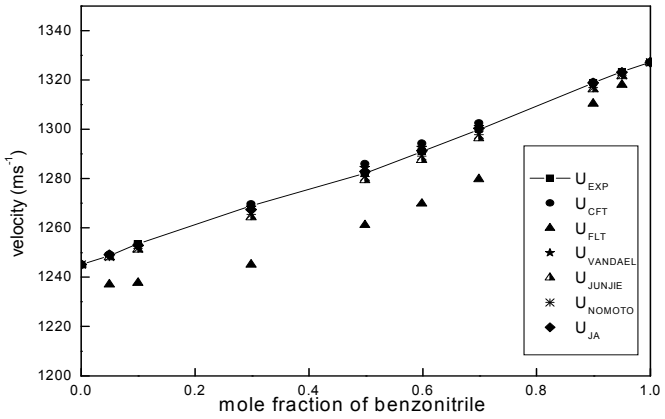

Fig. 1.7 (c). Variation of ultrasonic velocity with mole fraction of benzonitrile at 50^{0}C in the mixture: Benzonitrile + G (0.7219)

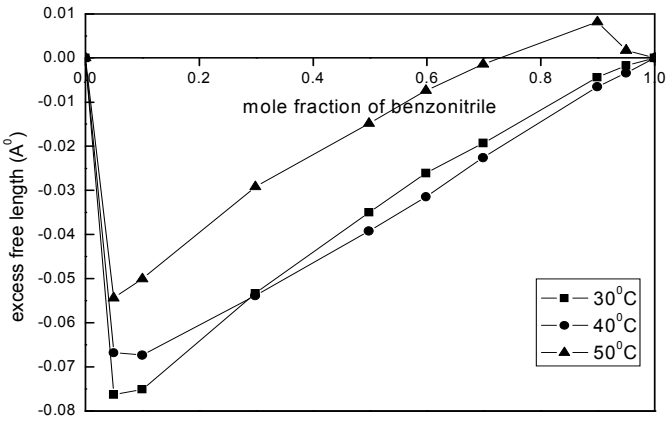

Fig. 2.1(c). Variation of excess free length with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

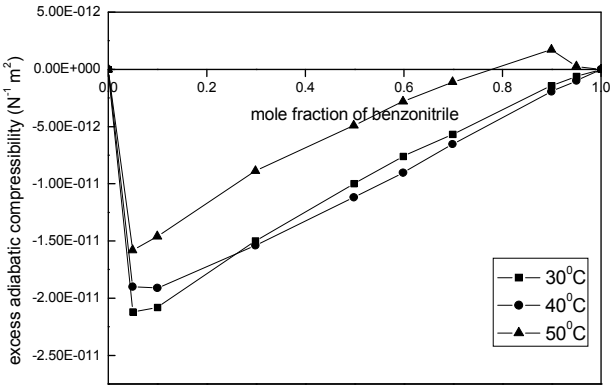

Fig. 2.1(a). Variation of excess adiabatic compressibility with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

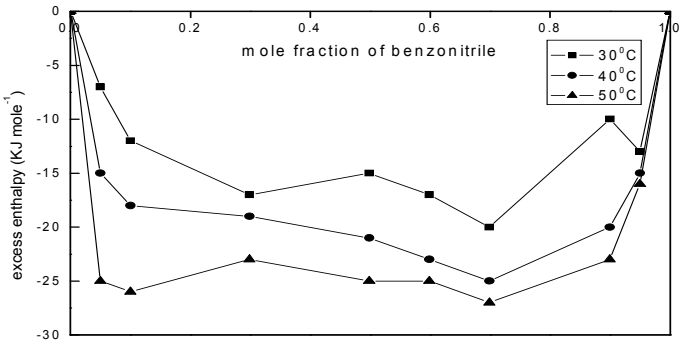

Fig. 2.1(d). Variation of excess enthalpy with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

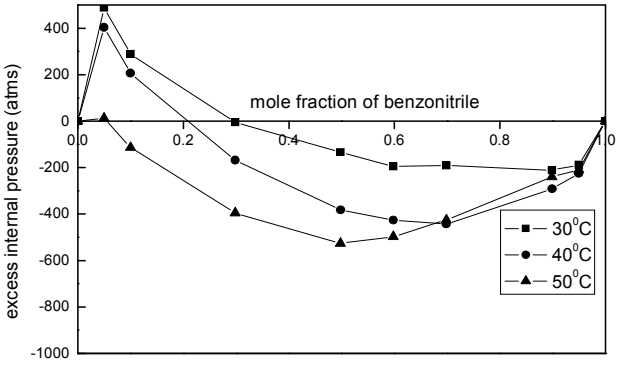

Fig.2.1(b). Variation of excess internal pressure with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

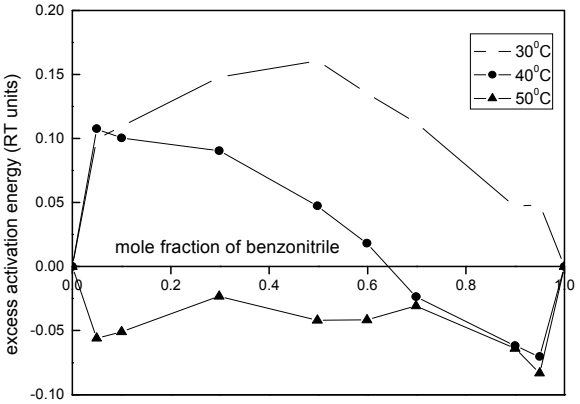

Fig. 2.1(e). Variation of excess activation energy with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

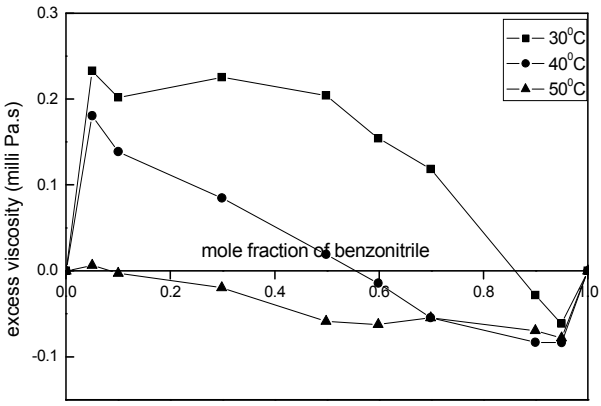

Fig. 2.1(f). Variation of excess viscosity with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

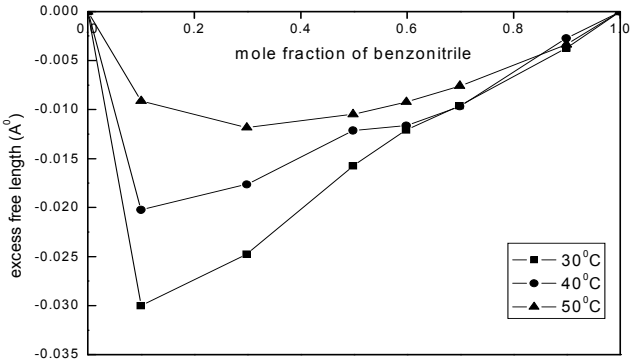

Fig. 2.2(c). Variation of excess free length with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

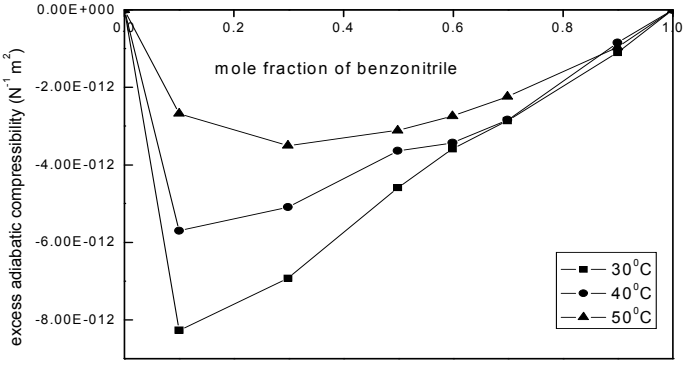

Fig. 2.2(a). Variation of excess adiabatic compressibility with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

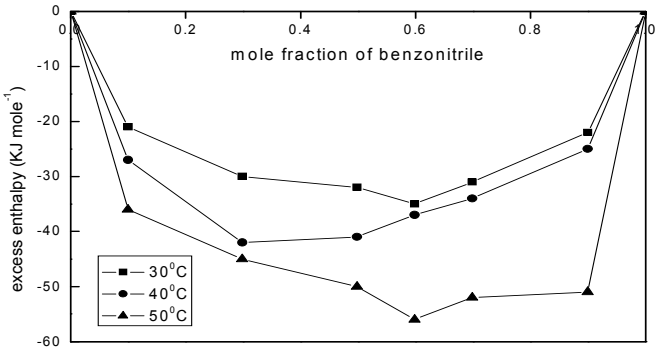

Fig. 2.2(d). Variation of excess enthalpy with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

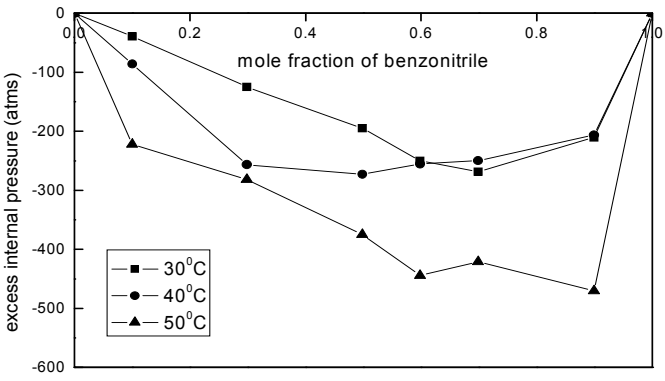

Fig. 2.2(b). Variation of excess internal pressure with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

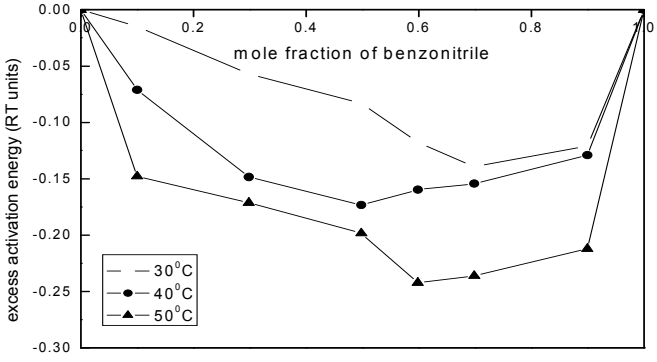

Fig. 2.2(e). Variation of excess activation energy with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

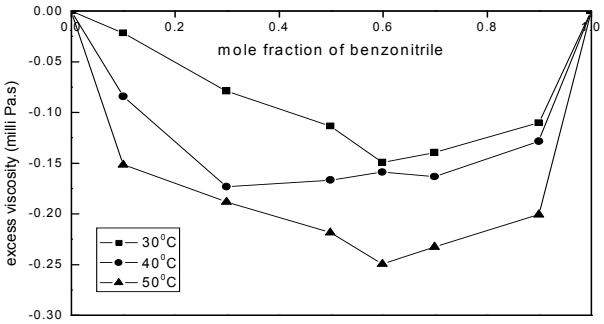

Fig. 2.2(f). Variation of excess viscosity with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

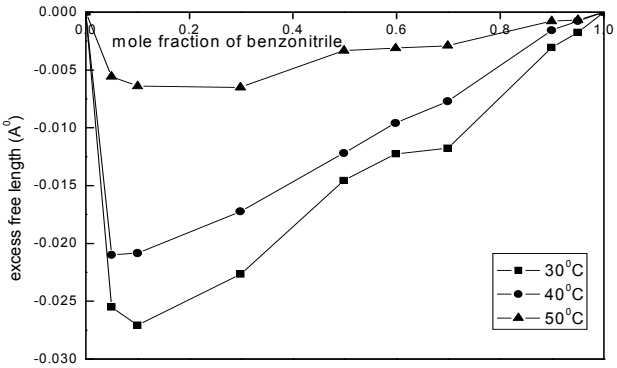

Fig.2.3(c). Variation of excess free length with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

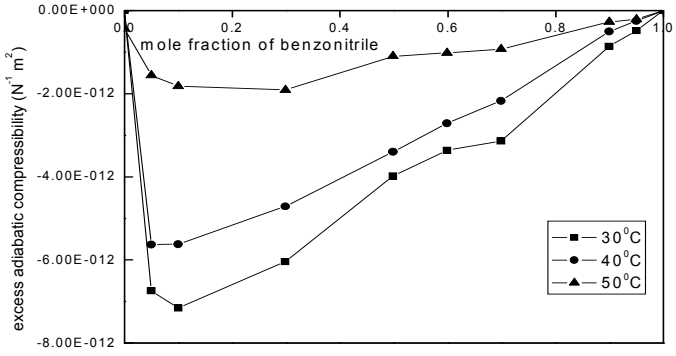

Fig. 2.3(a). Variation of excess adiabatic compressibility with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

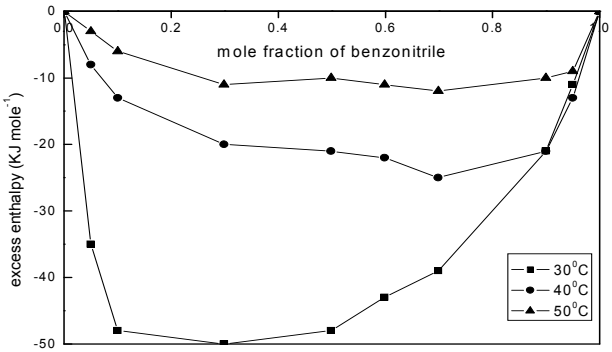

Fig. 2.3(d). Variation of excess enthalpy with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

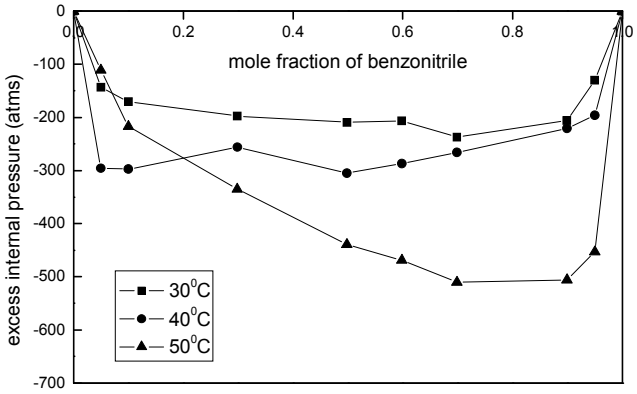

Fig. 2.3(b). Variation of excess internal pressure with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

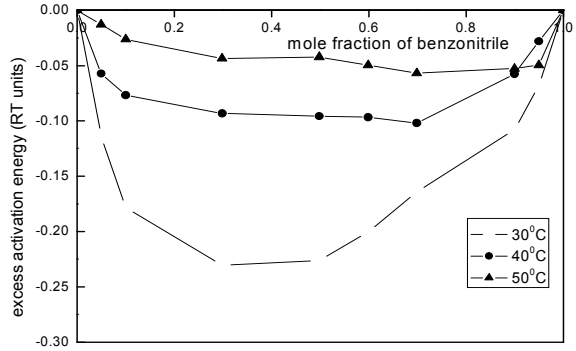

Fig. 2.3(e). Variation of excess activation energy with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

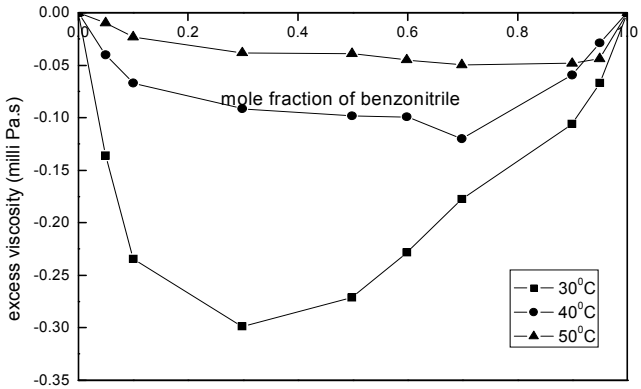

Fig. 2.3(f). Variation of excess viscosity with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

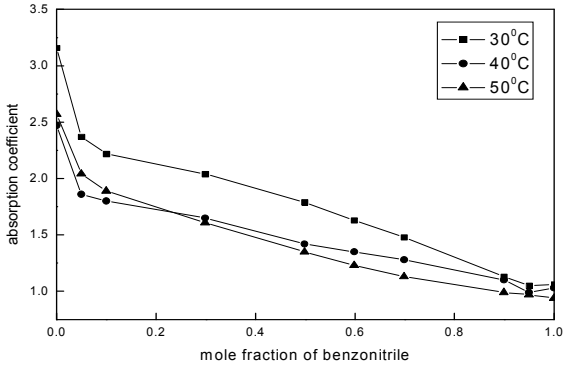

Fig. 3(c). Variation of absorption coefficient with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

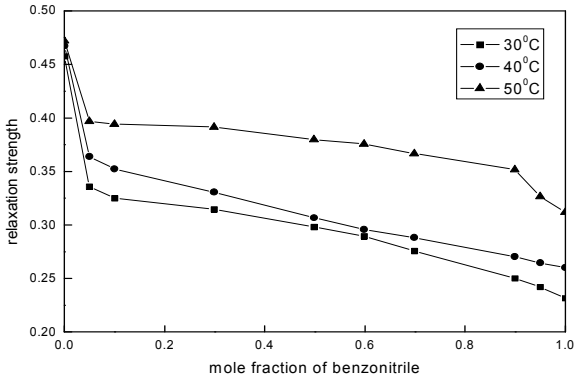

Fig. 3(a). Variation of relaxation strength with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

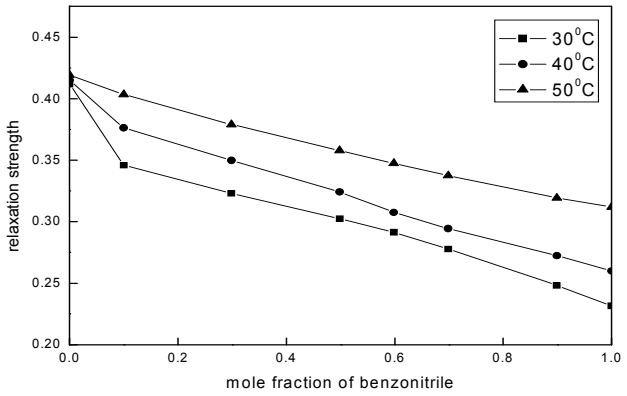

Fig. 4(a). Variation of relaxation strength with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

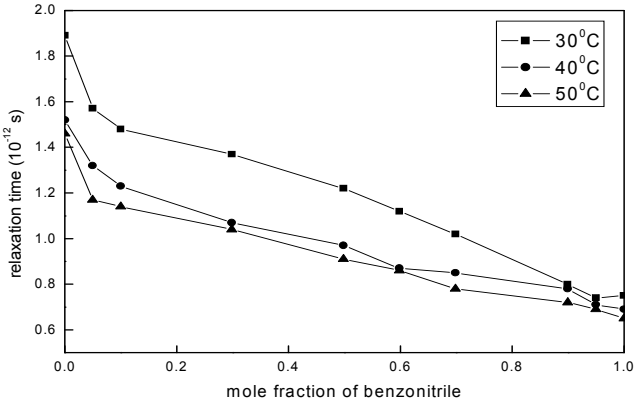

Fig.3(b). Variation of relaxation time with mole fraction of benzonitrile in the mixture: Benzonitrile + A (0.1760)

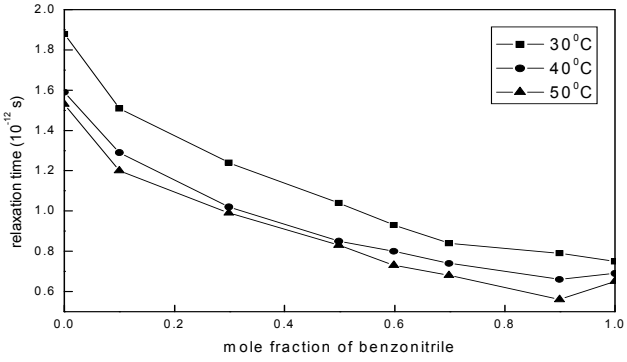

Fig. 4(b). Variation of relaxation time with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

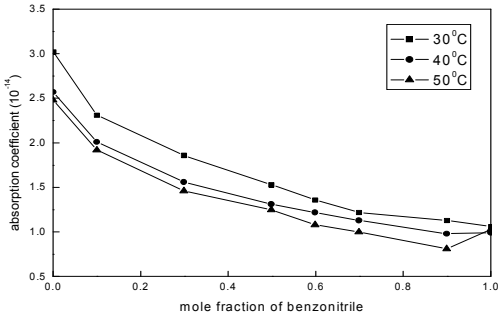

Fig. 4(c). Variation of absorption coefficient with mole fraction of benzonitrile in the mixture: Benzonitrile + E (0.5000)

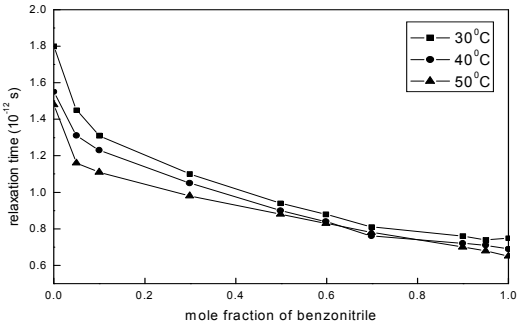

Fig. 5(b). Variation of relaxation time with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

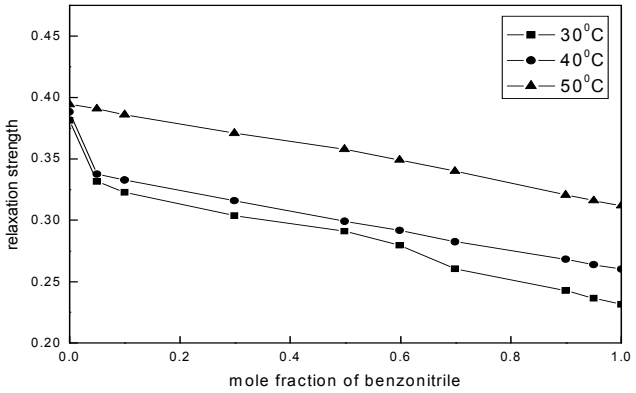

Fig. 5(a). Variation of relaxation strength with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

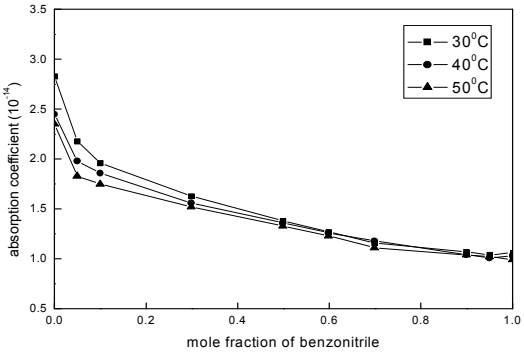

Fig. 5(c). Variation of absorption coefficient with mole fraction of benzonitrile in the mixture: Benzonitrile + G (0.7219)

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