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Thermodynamic and Transport Properties of Ternary Mixtures of 1-Butanol + 1, 2-Propanediol + Cyclohexanone at 308.15K, 318.15K and FT-IR Study

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Abstract: Density (ρ) and viscosity (η) for ternary liquid mixtures of 1-Butanol + 1,2-Propanediol + Cyclohexanone were measured at 308.15 and 318.15K over the entire range of composition. From the measured data, Excess volume (V^E), Deviation in viscosity (Δη) and excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) were calculated. The results were fitted with Redlich-kister's type polynomial equation and standard deviation between calculated and experimental excess parameter have been determined. Further, Heat of mixing and FT-IR spectrum are studied at equimolar concentration. The results provide information on the interaction of molecules in the pure liquids as well as in the ternary liquid mixtures.

Key words: Excess volume, Deviation in viscosity, Excess Gibbs free energy of activation of viscous flow, Heat of mixing, FT-IR spectra.

INTRODUCTION

Thermodynamic properties provide important information for the design of industrial separation processes and also give the knowledge about their intercomponent interaction in binary and ternary liquid mixtures [1]. The measurement of transport and thermodynamic properties of Alcohols, Alkanediols and Cyclohexanone (cyclic ketone) compounds have been employed in understanding the nature of molecular systems and physico-chemical behaviours of multicomponent liquid mixtures [2, 3]. Nature of excess properties of ternary liquid mixtures reflect difference in molecular size, shape and nature of interaction between the components [4]. This paper deals with the study of density(ρ) and viscosity(η) for the ternary system formed by 1-Butanol + 1,2-Propanediol + Cyclohexanone. Excess volumes (V^E) and deviation in viscosity (Δη), Gibbs free energies of activation of viscous flow (ΔG^{*E}) and molar volumes (V_{mix}) were calculated for the ternary mixtures and analysed to study the nature of molecular interaction between the components in the liquid mixtures.

This work involves systematic studies on thermodynamic properties of ternary liquid mixtures. The present work is focused on the qualitative explanation of the influence of molecular volumetric data of ternary mixtures containing1-Butanol, 1,2-Propanediol and Cyclohexanone. 1-Butanol (1) is considered as first component and second component is 1,2-Propanediol (2) and Cyclohexanone (3) as the third component. Moreover a survey of literatures has shown that the study on ternary liquid mixtures of 1-Propanol and 1,2-Propanediol with Cyclohexanone was reported earlier.

1-Butanol is polar and self associated molecules. Generally alkanols are used as fuels, perfumes, cosmetics, paints, vanishes, drugs, explosives, fats, waxes, resins, plastics and rubber, detergents etc. Alkanediols are self associated compounds through intermolecular hydrogen bonding with other molecules and also intramolecular hydrogen bonding within their molecules. Cyclohexanone is expected to exhibits dipole-dipole interaction in pure state because of its fairly high dipolemoment. However the association between Cyclohexanone molecules is weak and does not compete with high degree of association between alcohol molecules.

EXPERIMENTAL METHODS

The chemicals used in the present study are analytical grade (Merck) and further purified by standard methods [5, 6]. Before use the chemicals were dried by suitable drying agents to remove the water content, if any. The mixtures were prepared by knowing mass and were kept in special air tight glass stoppered conical type bottles to avoid evaporation. The weighing measurements were performed on a Shimasdzu Auy 220 Japan electronic digital balance with precision of ± 0.0001g was used for the mass measurements.

The density of pure liquids and their liquid mixtures were measured by using special type specific gravity bottle of 10ml capacity with an accuracy ± 0.0001g. The specific gravity bottle containing solution was immersed in a constant temperature water bath (Guna company) measured at 308.15 and 318.15K. Each reported values are the average of at least three measurements.

The viscosity of pure liquids and their liquid mixtures were measured by using an ostwald viscometer of 10ml capacity. The viscosities at temperature 308.15 and 318.15K were measured. The time is given to attain thermal equilibrium for the content of viscometer was 15min. The time of flow was measured with an accurate stop watch which is capable of measuring time to within 0.01s. Three sets of reading for the flow times were taken and the average values were taken for each pure liquids and liquid mixtures.

Heat of mixing of ternary liquid mixtures were measured with calorimeter (Dewar flask) at equimolar concentration.

IR study

IR spectra for pure liquids and their liquid mixtures at equimolar concentration were recorded by Brucker FT-IR, Alpha-E Germany.

Table - 1: Comparison of density (ρ) and viscosity (η) values with literature values of pure liquids at 308.15K and 318.15K

Name of the Components	Temperature K	Density ρ/g cm^{-3}		Viscosity η/mPa.s	
		Expt	Lit	Expt	Lit
1-BUTANOL	308.15	0.7970	0.7981[7]	1.7495	2.0120[8]
	318.15	0.7903	0.7902[9]	1.2645	1.583010]
1,2- PROPANEDIOL	308.15	1.0256	1.0251 [11]	21.3250	25.2200 [12]
	318.15	1.0199	1.0180 [13]	12.7391	12.7800 [14]
CYCLOHEXANONE	308.15	0.9290	0.9306 [15]	1.3140	1.6562 [16]
	318.15	0.9237	0.9225 [17]	1.0640	1.3700 [18]

RESULTS AND DISCUSSION

Comparison of experimental density (ρ) and viscosity (η) values with literature values for pure 1-Butanol, 1,2-Propanediol and Cyclohexanone are presented in Table-1. There is good agreement with literature values at 308.15 and 318.5K temperature for both density (ρ) and viscosity (η).

The densities (ρ) and viscosities (η) of given ternary mixtures containing namely 1-Butanol and 1,2-Propanediol with Cyclohexanone at 308.15 and 318.15K are presented in Table 2 and 3 which also includes the values of excess thermodynamic function viz., excess volume (V^E), deviation in viscosity (Δη), molar volume (V_{mix}) and excess Gibbs free energy of activation of viscous flow (ΔG^{*E}). It can be seen that variation of density (ρ) and viscosity (η) with composition of ternary mixture is non-linear which indication the presence of molecular interactions [19,20].

The excess volume of the given ternary liquid mixtures were evaluated from the molar volumes of mixtures and that of its pure components V_1, V_2 and V_3 using the equation (1) [21].

$$V^E = \left[\frac{x_1M_1 + x_2M_2 + x_3M_3}{r_{mix}}\right] - \left[\frac{x_1M_1}{r_1} + \frac{x_2M_2}{r_2} + \frac{x_3M_3}{r_3}\right] \quad \text{... (1)}$$

Viscosities of ternary liquid mixtures and their pure liquids were calculated by using the following equation (2) [21].

$$\eta = \left(At - B/t\right) \times r \quad \text{... (2)}$$

where A and B are characteristic constant, t is the time flow, ρ is the density.

The molar volumes (V_{mix}) of mixtures and their pure liquid components were calculated from the measured density (ρ_{mix}) and pure liquids (1, 2 and 3), ρ_1, ρ_2 and ρ_3 using the following equation (3) [22].

$$V_{mix} = \left[\frac{x_1M_1 + x_2M_2 + x_3M_3}{r_{mix}}\right] \quad \text{... (3)}$$

where x_1,x_2 and x_3 are the molefraction of the individual components and ternary liquid mixtures respectively, V_1 is M_1/r_1, V_2 is M_2/r_2 and V_3 is M_3/r_3, M_1, M_2 and M_3 are the molecular weight of the components 1, 2 and 3, ρ_1, ρ_2 and ρ_3 densities of the pure components 1,2 and 3 of the ternary liquid mixtures.

The deviation in viscosity (Δη) of the ternary liquid mixtures have been calculated from the observed viscosity of mixtures (η_{mix}) and that of its pure components using the equation (4) [23].

$$\Delta\eta = \eta_{mix} - \{x_1\eta_1 + x_2\eta_2 + x_3\eta_3\} \quad \text{... (4)}$$

where η_{mix} is the viscosity of ternary liquid mixtures and η_1, η_2 and η_3, are the viscosity of pure components respectively 1, 2 and 3, x_1, x_2 and x_3 are the mole molefraction of the components 1, 2 and 3.

Excess Gibbs energy of activation of viscous flow (ΔG^{*E}) for the liquid mixtures were computed from the following equation (5) [24].

$$\Delta G^{*E} = RT\left(\ln(\eta_{mix}V_{mix})\right) - [x_1\ln(\eta_1 v_1) + x_2\ln(\eta_2 v_2) + x_3\ln(\eta_3 v_3)] \quad \text{... (5)}$$

where the letters have their usual significance.

Grunberg and Nissan [25] put forward logarithmic relation between viscosity of binary mixtures and their pure components in equation (6).

$$\ln\eta_{mix} = x_1 \ln\eta_1 + x_2 \ln\eta_2 + x_1 x_2 d \quad \text{... (6)}$$

on applying to ternary liquid mixtures this equation take up the following form (7).

$$\ln\eta_{mix} = x_1\ln\eta_1 + x_2 \ln\eta_2 + x_3 \ln\eta_3 + x_1 x_2 x_3 d \quad \text{... (7)}$$

where d is constant regarded as a measure of strength of interaction between mixing component molecules.

Excess values of other parameter are calculated using the relation (8) [26].

$$A^E = A_{exp} - A_{id} \quad \text{... (8)}$$

$A_{id} = \Sigma x_i A_i$, x_i and A_i are the molefraction and parameters of the i^{th} component liquid.

All the calculated excess values were fitted to Redlich- kister type polynomial equation (9).

$$A^E = x_1, x_2 x_3 [a + b x_1 (x_2 - x_3) + c x_1^2 (x_2 - x_3)^2] \quad \text{... (9)}$$

by the method of least squares to derive the adjustable parameters a, b and c. From these a, b and c values, theoretical values for all the excess parameter were calculated using the following relation (10) [26].

$$\sigma = [(A^E_{exp} - A^E_{cal})^2 / (n - m)]^{1/2} \quad \text{... (10)}$$

where n is the number of measurements and m is the number of adjustable parameters. The values of a, b, c and σ are given in the Table 4(a) and 4 (b).

Table - 2: Densities, viscosities and Excess parameters for the ternary mixture of 1-Butanol + 1,2-Propanediol + Cyclohexanone at 308.15K

X_1	X_2	X_3	ρ g.cm^{-3}	V^E (cm^{3}mol^{-1})	η (mPa.s)	Δη (mPa.s)	Δlnη (mPa.s)	d	V_{mix} (cm^{3}mol^{-1})	V_1 (cm^{3}mol^{-1})	V_2 (cm^{3}mol^{-1})	V_3 (cm^{3}mol^{-1})	ΔG^{*E} (kJmol^{-1})
0.0985	0.2051	0.7059	0.9324	-0.0825	1.7075	-3.7661	-0.3403	-60.8526	98.7611	9.1603	15.2185	74.4652	11.3388
0.2038	0.2936	0.4974	0.9263	-0.1613	2.0333	-5.2378	-0.4385	-37.8693	93.0469	18.9531	21.7852	52.4706	11.9499
0.2929	0.4012	0.3051	0.9231	-0.2130	2.7296	-6.7392	-0.4705	-40.1298	88.9793	27.2393	29.7692	32.1849	12.6179
0.4035	0.4988	0.0995	0.9161	-0.3070	4.6121	-6.8613	-0.2504	-87.3124	84.7240	37.5249	37.0111	10.4962	13.4065
0.4528	0.1547	0.4018	0.8844	-0.1976	1.5385	-3.0805	-0.4055	-29.2845	95.7756	42.1098	11.4788	42.3857	11.2798
0.6047	0.2019	0.2033	0.8664	-0.2114	1.8235	-3.8070	-0.4107	-40.1528	92.4508	56.2363	14.9810	21.4460	11.3325
0.6926	0.2102	0.1013	0.8533	-0.1580	2.1419	-3.6853	-0.2965	-70.9945	90.5347	64.4109	15.5969	10.6861	11.5093
0.7960	0.1026	0.1023	0.8323	-0.1249	1.6761	-2.0388	-0.2706	-93.6935	92.3057	74.0270	7.61296	10.7916	11.3839
0.9042	0.0496	0.0509	0.8142	-0.0674	1.7872	-0.9192	-0.0907	-93.5414	93.0713	84.0894	3.6803	5.3694	11.0259
0.6953	0.1022	0.2024	0.8463	-0.0789	1.6658	-1.9959	-0.2465	-52.1157	93.5165	64.6620	7.5832	21.3511	11.5411
0.5038	0.2033	0.2927	0.8796	-0.1678	1.8512	-3.7501	-0.3679	-32.2001	92.6455	46.8527	15.0849	30.8768	11.7241
0.2887	0.3176	0.4094	0.9174	-0.2016	2.1379	-5.6779	-0.4852	-32.4087	93.3997	26.8487	23.5660	43.1875	12.1733
0.0969	0.3979	0.5052	0.9488	-0.1664	2.5515	-6.7670	-0.4729	-71.4336	91.6625	9.0115	29.5243	53.2934	12.7595
0.3992	0.4453	0.1526	0.9126	-0.3286	4.7554	-5.6394	-0.0682	-58.4375	85.9343	37.1250	33.0414	16.0977	13.4251
0.1976	0.5967	0.2122	0.9530	-0.2052	6.6399	-6.7092	-0.1011	-77.8149	84.8308	18.3765	44.2754	22.3849	14.7039
0.1065	0.7062	0.1911	0.9764	-0.1650	6.5032	-8.9939	-0.4003	-56.2498	82.2982	9.9043	52.4003	20.1590	14.5397
0.0994	0.8032	0.0973	0.9879	-0.13053	10.6481	-6.7818	-0.1744	-24.5892	78.9750	9.2440	59.5978	10.2641	15.7921
0.0652	0.8822	0.0525	1.0014	-0.0619	14.5615	-4.4344	-0.0718	-08.0633	76.9990	6.0635	65.4596	5.5382	15.3174
0.1806	0.7169	0.1025	0.9679	-0.2361	8.2287	-7.5097	-0.2149	-72.9094	80.5656	16.7955	53.1943	10.8127	14.3980
0.2971	0.5060	0.2022	0.9319	-0.2954	3.7883	-7.7875	-0.4377	-56.8868	86.2088	27.6299	37.5454	21.3300	13.3356
0.3938	0.3058	0.3020	0.9018	-0.1829	1.9795	-5.6274	-0.5555	-33.3702	90.9872	36.6229	22.6905	31.8579	11.8329
0.5007	0.1025	0.4017	0.8749	-0.2162	1.5821	-2.0074	-0.2445	-33.6598	96.3279	46.5644	7.6055	42.3752	11.0456
0.3977	0.1521	0.4503	0.8919	-0.2696	1.4280	-3.1029	-0.4545	-29.4108	95.5027	36.9856	11.2858	47.5020	11.5235
0.1944	0.2068	0.5988	0.9218	-0.2267	1.6458	-3.8910	-0.4067	-37.0973	96.3635	18.0789	15.3446	63.1672	11.9477
0.1881	0.1142	0.6944	0.91535	-0.1485	1.4230	-2.2537	-0.2914	-42.8393	99.0696	17.4930	8.4736	73.2520	11.2758
0.1058	0.1017	0.7963	0.9242	-0.1005	1.6078	-1.7923	-0.1129	-68.1306	101.2860	9.8392	7.5461	84.0015	11.5477
0.0512	0.0538	0.8955	0.9271	-0.0560	1.3548	-1.0586	-0.1340	-77.1792	103.1633	4.7615	3.9919	94.4660	11.0784

Table - 3: Densities, viscosities and Excess parameters for the ternary mixture of 1-Butanol + 1,2-Propanediol + Cyclohexanone at 318.15K

X_1	X_2	X_3	ρ g.cm^{-3}	V^E (cm^{3}mol^{-1})	η (mPa.s)	Δη (mPa.s)	Δlnη (mPa.s)	d	V_{mix} (cm^{3}mol^{-1})	V_1 (cm^{3}mol^{-1})	V_2 (cm^{3}mol^{-1})	V_3 (cm^{3}mol^{-1})	ΔG^{*E} (kJmol^{-1})
0.0985	0.2051	0.7059	0.9269	-0.0933	1.40800	-2.0804	-0.2466	-40.9470	99.3403	9.2380	15.3035	74.8924	11.0830
0.2038	0.2936	0.4974	0.9208	-0.1904	1.6222	-2.9049	-0.3420	-27.2627	93.6013	19.1138	21.9070	52.7716	11.9476
0.2929	0.4012	0.3051	0.9173	-0.2359	2.1672	-3.6386	-0.3351	-30.1470	89.5384	27.4702	29.9356	32.3696	11.5129
0.4035	0.4988	0.0995	0.9102	-0.3423	3.5577	-3.4125	-0.1010	-67.1495	85.2738	37.8431	37.2180	10.5564	12.6504
0.4528	0.1547	0.4018	0.8786	-0.2230	1.2630	-1.7078	-0.2913	-18.4143	96.4146	42.4668	11.5429	42.6289	10.9413
0.6047	0.2019	0.2033	0.8605	-0.2510	1.5505	-2.0024	-0.2296	-26.4861	93.0947	56.7131	15.0648	21.5691	11.7993
0.6926	0.2102	0.1013	0.8470	-0.1816	1.7643	-1.8969	-0.1359	-47.1489	91.2057	64.9569	15.6841	10.7474	11.2645
0.796	0.1026	0.1023	0.8260	-0.1465	1.4218	-1.0005	-0.1022	-54.0159	93.0162	74.6545	7.6555	10.8535	11.8126
0.9042	0.0496	0.0509	0.8077	-0.0842	1.4229	-0.4064	0.0111	-149.2755	93.8187	84.8023	3.70091	5.4002	11.0240
0.6953	0.1022	0.2024	0.8399	-0.0815	1.2416	-1.1548	-0.2193	-30.0837	94.2268	65.2102	7.6256	21.4736	10.0334
0.5038	0.2033	0.2927	0.87367	-0.1913	1.4332	-2.1050	-0.2937	-21.4459	93.2806	47.2499	15.1692	31.0540	11.0610
0.2887	0.3176	0.4094	0.9117	-0.2253	1.6795	-3.1670	-0.3827	-23.4925	93.9831	27.0763	23.6977	43.4353	11.8277
0.0969	0.3979	0.5052	0.9435	-0.1960	1.8139	-3.9150	-0.4711	-54.1619	92.1800	9.0879	29.6893	53.5992	11.1317
0.3992	0.4553	0.1526	0.9077	-0.3627	3.4764	-2.9907	-0.0157	-44.2451	87.2382	37.4398	33.9722	16.1901	12.6440
0.1976	0.5967	0.2122	0.9475	-0.24404	5.0871	-2.9899	0.0487	-61.4404	85.3237	18.5323	44.5228	22.5133	13.7766
0.1052	0.7062	0.1911	0.9712	-0.1926	4.8697	-4.4629	-0.2505	-127.5682	82.6412	9.8664	52.6932	20.2747	13.0569
0.0994	0.8032	0.0973	0.9824	-0.1532	7.7500	-2.7112	-0.0255	-264.8396	79.4226	9.3224	59.9308	10.3230	14.6968
0.0652	0.8822	0.0525	0.9959	-0.0836	10.8735	-0.5031	0.1228	-747.1642	77.4263	6.1149	65.8254	5.5699	15.8007
0.1806	0.7169	0.1025	0.9622	-0.2550	6.0377	-3.4323	-0.074	-139.3393	81.0484	16.9379	53.4916	10.8747	14.4938
0.2971	0.506	0.2022	0.9263	-0.3352	2.9611	-4.0756	-0.2843	-43.9800	86.7354	27.8641	37.7552	21.4524	12.8705
0.3978	0.3058	0.302	0.8956	-0.2168	1.6498	-3.0700	-0.3895	-23.7320	91.9485	37.3085	22.8173	32.0407	11.9270
0.5007	0.1025	0.4017	0.8696	-0.3141	1.3032	-1.0630	-0.1383	-19.2953	96.9104	46.9592	7.6480	42.6183	10.7701
0.3977	0.1521	0.4503	0.8858	-0.2682	1.2010	-1.7185	-0.3250	-18.4780	96.1533	37.2991	11.3489	47.7746	10.7396
0.1944	0.2068	0.5988	0.9158	-0.2029	1.3911	-2.1262	-0.2789	-24.9683	96.9887	18.2322	15.4304	63.5297	11.2673
0.1881	0.1142	0.6944	0.9099	-0.1715	1.1589	-1.2725	-0.2302	-25.1817	99.6626	17.6413	8.5210	73.6724	10.7421
0.1058	0.1017	0.7963	0.9191	-0.13851	1.2837	-0.9928	-0.0832	-38.6178	101.8556	9.9226	7.5883	84.4834	11.5548
0.0512	0.0538	0.8955	0.9218	-0.0647	1.1741	-0.5287	-0.0439	-82.7319	103.7593	4.8019	4.0142	95.0081	10.9488

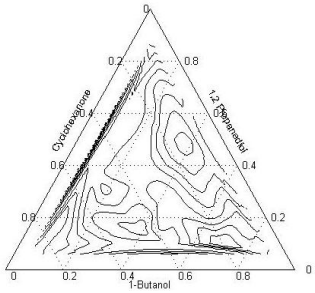

Fig. 1 (a) : Contour curves of Excess volume Versus molefraction x_1, x_2 and x_3 ternary mixtures of 1-Butanol + 1, 2-Propanediol + Cyclohexanone at 308.15K

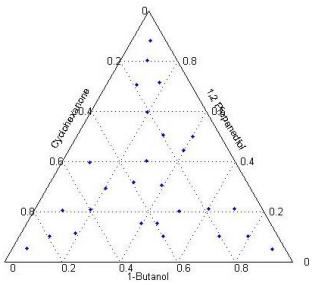

Fig. 1 (b) : Contour curves points of Excess volume Versus molefraction x_1, x_2 and x_3 ternary mixtures of 1-Butanol + 1, 2- Propanediol + Cyclohexanone at 308.15K

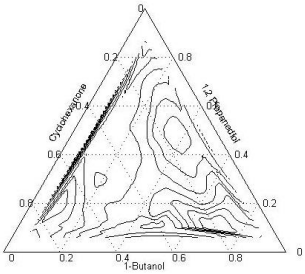

Fig. 2 (a) : Contour curves of Excess volume Versus molefraction x_1, x_2 and x_3 ternary mixtures of 1- Butanol + 1, 2- Propanediol + Cyclohexanone at 318.15K

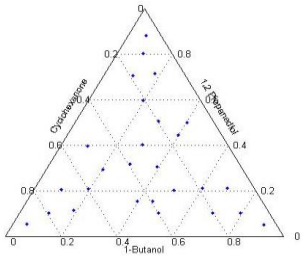

Fig. 2 (b) : Contour curves points of Excess volume Versus molefraction x_1, x_2 and x_3 ternary mixtures of 1-Butanol + 1,2-Propanediol+Cyclohexanone at 318.15K

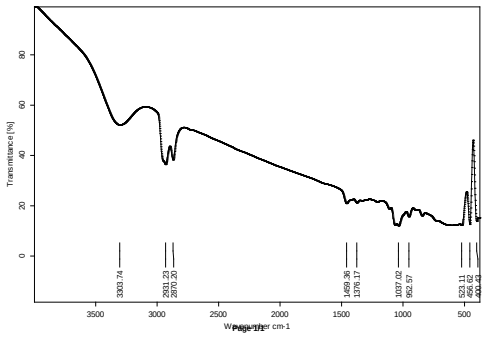

Fig. 3: FT – IR Spectra of 1-Butanol

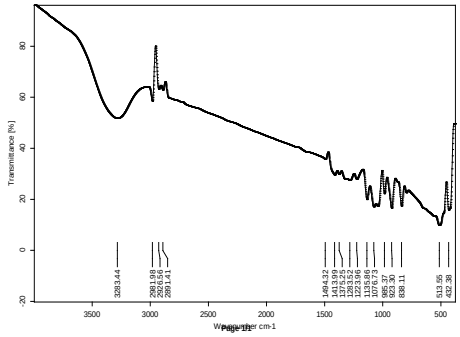

Fig. 4: FT-IR spectra of 1,2-Propanediol

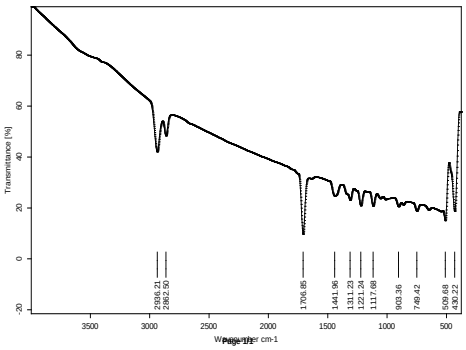

Fig. 5: FT-IR spectra of Cyclohexanone

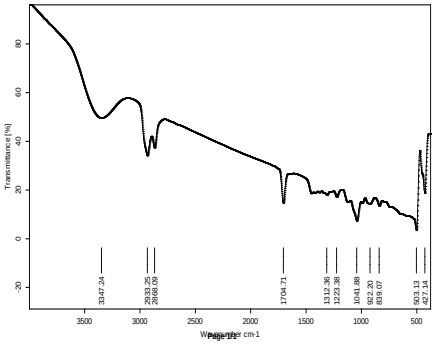

Fig. 6: FT-IR spectra of 1-Butanol +1,2-Propanediol + Cyclohexankone at equimolar concentration.

Table - 4(a): Adjustable parameters a, b, c and σ (standard deviation) values for the excess parameters at 308.15K

Parameters	a	b	c	σ
V^E (g.cm^{-3})	-6.3447	-14.3846	-313.9800	0.0024
Δη (mPa.s)	-194.0760	-818.7940	-542.0180	0.1083
Δ^{G*E} (kJmol^{-1})	457.5170	471.8050	6860.8700	0.5228

Table - 4(b): Adjustable parameters a, b, c and σ (standard deviation) values for the excess parameters at 318.15K

Parameters	a	b	c	σ
V^E (g.cm^{-3})	-7.3429	-15.9020	-348.1690	0.00291
Δη (mPa.s)	-03.7660	-367.0470	11.9286	0.0359
Δ^{G*E} (kJ mol^{-1})	434.9310	492.6480	7073.5900	0.4985

An examination of data in the Table – 2 and 3 shows that the variation of excess volume (V^E) are negative over entire composition rage at 308.15K and 318.15K. The negative values of excess volume (V^E) are plotted against with molefractions x_1, x_2 and x_3. These are graphically (displayed) represented as 3D contour diagram in Fig 1(a), 1(b), 2(a) and 2(b). In the present investigated system containing namely 1-Butanol + 1,2-Propanediol + Cyclohexanone a reduction in volume take place during mixing of liquids. The change in volume on mixing is discussed on the basis of the following type of interactions. (i) breaking of hydrogen bonds on self associated liquids (ii) formation of new H-bond between 1-Butanol + 1,2-Propanediol is due to proton donating and proton accepting nature of self associated 1-Butanol and 1,2-Propanediol . (iii) dipole-dipole interaction operating through 1-Butanol + Cyclohexanone and 1,2-Propanediol + Cyclohexanone. The negative values of v^E predict that there is presence of specific attractive interaction among unlike molecules.

The experimental data V^E of constitute binary mixtures are negative and the v^E values are reported by Mohammed Almasi et al. [27] for 1-Butanol +1,3-Propanediol at 303.15K are negative and Tsierkezos et al. [28] were reported the v^E values are negative for 1-Butanol + Cyclohexanone at 293.15K. Whereas present investigation are found to be same negative v^E value when performed at 308.15K and 318.15K. The excess

volume (V^E) values becomes more negative with increasing temperature. According to Rastogi et al. [29] as temperature increases, the thermal energy activate the molecules and increase the rate of association of unlike molecules. Hence the interaction increases with increasing temperature. Therefore a heteroassociation are formed in 1-Butanol + 1,2-Propanediol + Cyclohexanone ternary system.

The deviation in viscosity for the mixtures of 1-Butanol + 1,2-Propanediol + Cyclohexanone at 308.15K and 318. 15K are presented in Table -2 and 3. It is observed that the value of Δη are negative over the whole concentration range. The negative Δη values can be interpreted qualitatively by considering the strength of intermolecular hydrogen bonding, molecular size, shape of the molecules, viscous nature of mixtures and pure liquids [30]. The Δlnη and Grunberg Nissan interaction parameter d are also negative values. The negative values of Δη are decreased with increasing temperature from 308.15K to 318.15K. This suggest that the given mixture is less viscous and can flow more easily than the corresponding pure liquids.

Excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) are positive at 308.15K and 318.15K which are presented in Table - 2 and 3. The positive value ΔG^{*E} may be due to size effect and as reliable measure to detect the presence of interaction between the molecules [31]. As temperature is raised from 308.15K to 318.15K, this positive values of ΔG^{*E} are decreased in the present system. The decreasing the values of ΔG^{*E} with increasing temperature predicts that there will be specific interaction between the component molecules.

HEAT OF MIXING

The heats of mixing value of the given ternary system were measured with calorimeter. Generally heat of mixing of binary and ternary liquid mixture may be influenced by two factor such as (i) The absorption of heat [endothermic] due to the dissociation of self associated liquids. (ii) The second factor is the liberation of heat [Exothermic] as result of hydrogen bonding formation between the component molecules [32]. The heat of mixing value of the ternary mixture at near equimolar concentration is -993.24J/mol. The observation of V^E, Δη, ΔG^{*E} and ΔH^E_{mix} would predicts that there is specific interaction between the component molecules.

FT-IR SPECTRA

FT-IR spectra of pure liquids of 1-Butanol, 1,2-Propanediol, Cyclohexanone and mixtures of 1-Butanol + 1,2-Propanediol + Cyclohexanone at equimolar concentration are depicted in Figures (3,4,5 and 6). According to Karunakar and Srinivas [33] the intensity of an absorption in the IR spectrum is related to change in dipolemoment that occurs during the vibration. Consequently, vibration that (occur) produce large change in dipolemoment results in more intense absorption than those that result in a relatively modest change in dipole. Vibration that do not change in dipolemoment will show little or no absorption for this vibration. Further FT-IR spectra has been used extensively to study intermolecular and intramolecular hydrogen bonding interaction between the component molecules. Usually intermolecular hydrogen bonding gives rise to broad bands, where as intramolecular hydrogen bonds appears sharp bands. Alcoholic OH band appears at 3650cm^{-1} which is due to free-OH group in their pure state.

Pure 1-Butanol exhibits peak of 3303.74 cm^{-1} and 1,2-Propanediol exhibits 3283.44cm^{-1}, no-OH peak can be observed for Cyclohexanone. When 1-Butanol is mixed with 1,2-Propanediol and Cyclohexanone mixture the absorption is shifted to longer wave number caused by strong intermolecular interaction like hydrogen bonding between OH group of 1-Butanol and OH-group of 1,2-propanediol. It is clearly observed, the mixtures has peak at 3347.24cm^{-1} and the spectrum is broad. This supports the formation of intermolecular hydrogen bonding between the component molecules.

CONCLUSION

The densities and viscosities for ternary liquid mixtures of 1-Butanol and 1,2-propanediol with cylohexanone are determined experimentally, at 308.15 and 318.15K over the whole composition range. The value of V^E, Δη and ΔG^{*E} are calculated from experimental results at both temperatures. The excess, deviation functions are fitted to Redlich-kister type polynomial equation and corresponding standard deviations are calculated. The observed negative value of V^E, Δη and the positive values of ΔG^{*E} for the given analysed ternary mixtures having the following conclusions may be drawn.

1. The negative magnitude of V^E values predicts attractive interactions are dominant over the repulsive force between the molecules. It is like that intermolecular H-bonding and dipole-dipole interaction between the molecules. This kind of interaction increasing with increasing temperature.
2. From Δη values suggest-that the given mixtures is less viscous and greater fluidity than that of corresponding pure liquids.

3. The values of ΔG^{*E} reveals that there would be specific interaction between the component molecules.
4. H^{E}_{mix} values reveals that attractive interaction among the unlike molecules.
5. FT-IR spectra observation, suggest that the formation of intermolecular hydrogen bonding between the component liquids.

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