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Molecular Interaction Study of Binary Solutions of n-Butyl Acetate and Isopropanol at Various Temperatures

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Abstract: *This paper presents molecular interaction studies of binary solutions of n-butyl acetate and isopropanol over the temperature range from 305K to 320 K at atmospheric pressure. Excess molar volume (V_m^E) and deviation in viscosity ($\Delta\eta$) were calculated using experimental density and viscosity data of binary solutions studied. Breaking of hydrogen bond of isopropanol molecules by the addition of ester leads to positive excess molar volume and negative deviation in viscosity contribute to weak dipole-dipole interaction and dispersion forces. Positive excess molar volume and negative deviation in viscosity are fitted in Redlich-Kister polynomial equation to validate the correctness of the experimental value. It is observed that excess molar volume increases with increasing temperature and it may be ascribable to dispersion forces. Experimental and calculated quantities used to interpret concerning possible molecular interactions in binary solutions of ester and isopropanol.*

Keywords: *Binary solution, Densities, deviation in viscosity, molecular interaction, viscosity, Redlich-Kister.*

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I. Introduction

Esters and alcohols are important chemicals which are widely used in chemical industries and knowledge of molecular interactions[1] help us to understand various systems during the industrial process. Esters comprise for strong fragrance, mainly involved in manufacturing of flavoured compounds [2] and fragrance industries[3] while alcohol is good solvent for different organic substances. Thermo-physical properties[4] of esters and alcohols achieved considerable interest of researchers due to its theoretical and practical applications. Information about molecular interaction of binary mixtures [5]of ester and alcohol can be obtained from the study of densities and viscosities [6]of binary solutions and is useful for various fields like pharmaceutical, production of bio-fuel[7], design of chemical plant and bio molecular [8] systems etc. Literature survey reveals that study on aliphatic esters in aqueous medium are abundant, but there is only few work is reported in the field of molecular interaction studies involving esters in non-aqueous medium. Therefore present work is aimed to investigate the molecular interaction behaviour of non-aqueous systems having ester as one component. Molecular interaction in binary system is governed by determination of excess molar volume and deviation in viscosity. Objective of the present work is to evaluate the excess parameters and understand the nature of interaction between ester and alcohol molecules in the binary solutions.

II. Experimental

Materials: n-butyl acetate and iso propyl alcohol were supplied by Loba Company. Purity of the chemicals is 99%. In the present work, both the chemicals were used without any further purification and the reagents were kept in air tight bottles in a desiccator.

Apparatus and Method: Mass measurements were done on electronic balance GC- 103 with accuracy 0.0001 kg. Pycnometer is used to measure density. Viscosities of the solutions were measured by Ostwald's Viscometer and thermostat is used to maintain the temperature. Time of flow of liquid is noted using electronic digital watch. The binary solutions of varying composition (0.1 to 1.0 M) were prepared and kept in air tight bottles at dry place. The densities and viscosities of solutions prepared were measured on the same day of preparation. All measurements performed thrice and average values are taken as final value.

III. Result and Discussion

Density

Measured densities of binary solutions of n-butyl acetate (1) and iso- propanol (2) at T = (305 to 320K) in overall composition range studied are listed in Table 1 and plotted in Fig 1.

Table – 1: Densities of binary solutions of n-butyl acetate (1) and isopropanol (2) at 305 to 320 K

Mole Fraction	Densities of binary solutions (in gm/cm^3)			
X1	**305 K**	**310 K**	**315 K**	**320 K**
0	0.7806	0.7768	0.7724	0.7692
0.1	0.7914	0.7856	0.7795	0.7743
0.2	0.7992	0.7931	0.7867	0.7811
0.3	0.8064	0.7994	0.7925	0.7874
0.4	0.8136	0.8065	0.8000	0.7944
0.5	0.8219	0.8146	0.8082	0.8024
0.6	0.8337	0.8259	0.8190	0.8128
0.7	0.8448	0.8367	0.8297	0.8238
0.8	0.8548	0.8473	0.8407	0.8345
0.9	0.8625	0.8557	0.8503	0.8444
1	0.8685	0.8628	0.8591	0.8547

As shown in Table 1 and Fig 1, densities of binary solutions increases with increasing mole fraction of ester at a particular temperature[9] and values of density decreases with increasing temperature at same mole fraction.

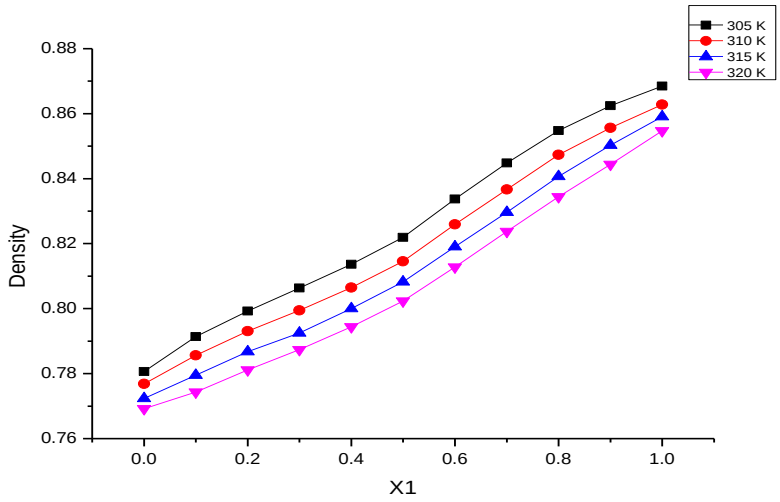

Fig: 1 Plot of density v/s X1 for n- butyl acetate and isopropanol

Excess molar volume

Experimental densities utilized to evaluate excess molar volume using equation (1) and listed in Table 2. Plot of excess molar volume v/s X1 is shown in Fig 2.

$$V_m E = \frac{X1M1 + X2M2}{\rho 12} - \left(\frac{X1M1}{\rho 1} + \frac{X2M2}{\rho 2}\right) \ldots\ldots\ldots\ldots\ldots (1)$$

Where ρ12 densities of solution, X1, M1, ρ1 and X2, M2, and ρ2 are mole fraction, molecular mass and density of n- butyl acetate (1) and iso-propanol (2) respectively.

Table-2: Excess Molar Volume of binary solutions of n-butyl acetate (1) and isopropanol (2) at 305 to 320 K

	Excess molar volume of binary solutions (in cm^3/mol)			
X1	**305 K**	**310 K**	**315 K**	**320 K**
0	0.0000	0.0000	0.0000	0.0000
0.1	0.3601	0.5422	0.7383	0.9461
0.2	0.8887	1.1043	1.3539	1.6095
0.3	1.3762	1.6734	2.0237	2.2262
0.4	1.7368	2.0564	2.3819	2.6398
0.5	1.8582	2.1962	2.5320	2.8212
0.6	1.3898	1.7709	2.2007	2.5270
0.7	0.8690	1.2893	1.7501	2.0228
0.8	0.3845	0.6849	1.1117	1.4162
0.9	0.1111	0.3022	0.5457	0.7946
1	0.0000	0.0000	0.0000	0.0000

Excess molar volume for the binary solutions of ester and alcohol found positive in whole range of composition(X1) and temperature range from 305 to 320 K. At a specified temperature, the values of excess molar volume increases on increasing composition of ester (1) up to X1= 0.5 and decreases on further increase of X1. Isopropanol is associated by hydrogen bonding and when ester is employed in solution, breaking of self-associated molecules takes place which may lead to positive excess molar volume[10]. Increase in excess molar volume with increasing temperature is assignable to dispersion forces [11].

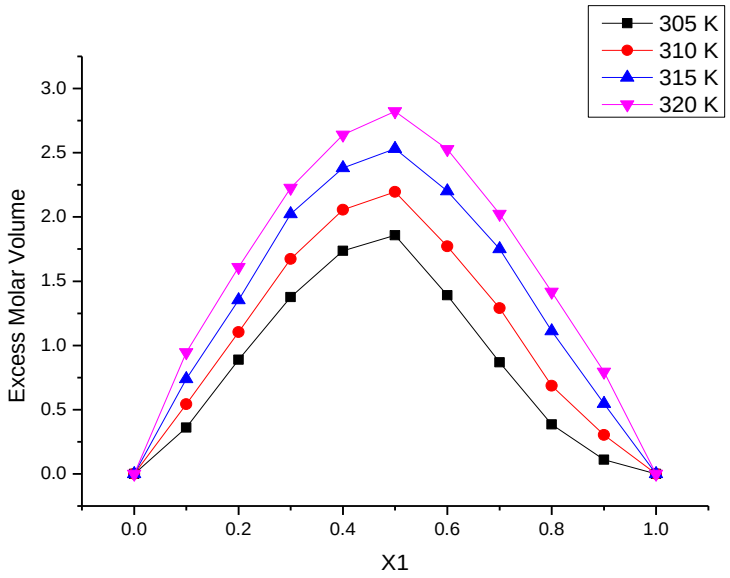

Fig: 2 Plot of Excess Molar Volume v/s X1 for n- butyl acetate and isopropanol

Viscosity

Experimental viscosities of binary solution of n- butyl acetate (1) and isopropanol (2) at 305, 310, 315 and 320K are enlisted in Table 3 and frame in Fig 3.

Table-3: Viscosities of binary solutions of n-butyl acetate (1) and isopropanol (2) at 305 to 320 K

Mole fraction	**Viscosities of binary solutions η (m.Pa.s)**			
X1	**305 K**	**310 K**	**315 K**	**320 K**
0	1.7312	1.6655	1.5713	1.4730
0.1	1.5765	1.5182	1.4326	1.3439
0.2	1.4380	1.3816	1.3031	1.2196
0.3	1.3091	1.2560	1.1766	1.1009
0.4	1.1848	1.1351	1.0620	0.9864
0.5	1.0730	1.0265	0.9586	0.8883
0.6	0.9820	0.9312	0.8683	0.8026
0.7	0.8956	0.8479	0.7884	0.7270
0.8	0.8136	0.7682	0.7125	0.6551
0.9	0.7428	0.6928	0.6407	0.5811
1	0.6688	0.6143	0.5599	0.4987

As mentioned in Table 3 and Fig 3, it is recognized that the viscosities of binary solutions decrease with increasing mole fraction of ester at same temperature and again it is found to be decreasing with increasing temperature at fixed mole fraction [11].

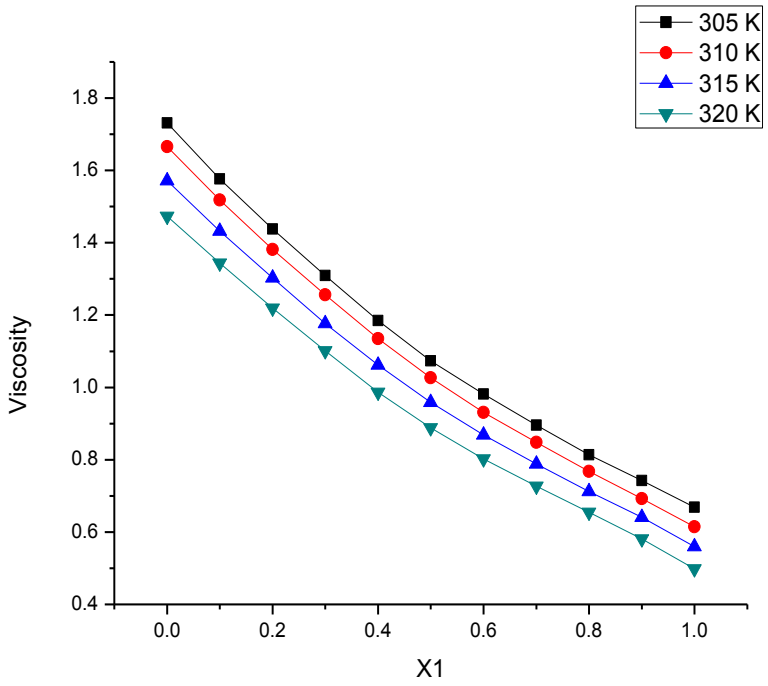

Fig: 3 Plot of Viscosity v/s X1 for n- butyl acetate and isopropanol

Deviation in viscosity

Viscosity data used to evaluate deviation in viscosity which is listed in Table 3 and plotted in Fig 3. Following equation is used to calculate deviation in viscosity in binary solution.

$$\Delta\eta = \eta 12 - (X1.\eta 1 + X2.\eta 2) \ldots\ldots\ldots\ldots (2)$$

Where $\Delta\eta$ is viscosity deviation, $\eta 12$ is viscosity of binary liquid solution, X1,$\eta 1$ and X2, $\eta 2$ are mole fraction and viscosity of component 1 and 2 respectively.

Table-4: Deviation in viscosities of binary solutions of n-butyl acetate (1) and isopropanol (2) at 305 to 320 K

Mole Fraction	**Deviation in viscosity Δη (m.Pa.s)**			
X1	**305 K**	**310 K**	**315 K**	**320 K**
0	0.0000	0.0000	0.0000	0.0000
0.1	-0.0485	-0.0422	-0.0376	-0.0317
0.2	-0.0807	-0.0737	-0.0660	-0.0585
0.3	-0.1034	-0.0941	-0.0913	-0.0798
0.4	-0.1215	-0.1099	-0.1047	-0.0968
0.5	-0.1270	-0.1134	-0.1070	-0.0975
0.6	-0.1118	-0.1036	-0.0962	-0.0858
0.7	-0.0920	-0.0817	-0.0749	-0.0640
0.8	-0.0677	-0.0564	-0.0497	-0.0385
0.9	-0.0323	-0.0267	-0.0204	-0.0150
1	0.0000	0.0000	0.0000	0.0000

Negative values of $\Delta\eta$ found in the case of all binary solutions of n- butyl acetate (1) and iso-propanol (2) over the entire range of composition. In the presence of ester, breaking of dipolar attraction of alcohol molecules occurs and this leads to negative deviation in viscosity [12][13] . Negative deviation in viscosity values[14] decrease with increment of temperature [15].

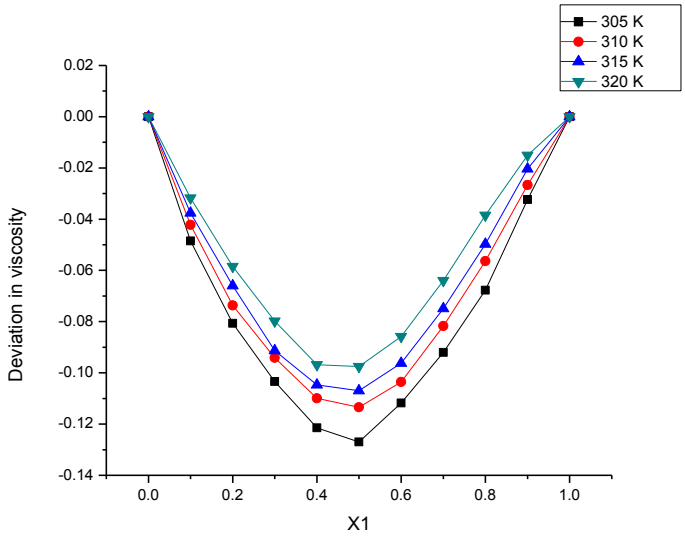

Fig: 4 Plot of Deviation in viscosities v/s X1 for n- butyl acetate and isopropanol

Redlich-Kister Ploynomial equation

Excess molar volume and deviation in viscosity are fitted in Redlich-Kister [16] polynomial equation and correlated [17]the experimental data.

$$Y = X1.X2\sum_{i=0}^{n} A_i\ (X1 - X2)^i \ \ldots\ldots\ldots\ldots (3)$$

Y is excess parameter[18], X1 and X2 are mole fractions of component 1 and 2 respectively. Ai is adjustable parameters obtained by fitting. The magnitude of correlation is evaluated by calculating standard deviation using equation (4). Fitting parameters and standard deviation given in Table 5.

$$\sigma = \sqrt{\frac{\Sigma\ (Y_{exp} - Y_{cal})^2}{(N - n)}} \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

σ Standard deviation, N are number of data points in the experiment and n is number of fitting parameters.

Table-5: Adjustable parameters and standard deviation of the Redlich-Kister polynomial equation for binary solution of n-butyl acetate (1) and isopropanol (2).

	T/K	A0	A1	A2	A3	A4	σ
V_m^E	**305**	7.1921	-0.021	-2.826	2.015	-6.0201	0.098727
	310	8.4146	-0.0011	-3.0441	1.841	-5.101	0.09877
	315	9.7032	-0.005	-3.8808	2.4241	-1.0208	0.09749
	320	10.7132	-0.002	-2.0106	2.7338	-1.0006	0.097378
Δη	**305**	-0.5002	0.0044	0.131	0.011	0.0466	0.008947
	310	-0.4541	0.0025	0.112	0.0128	0.0466	0.008746
	315	-0.4432	0.0014	0.211	0.0146	0.0472	0.009896
	320	-0.4001	0.0012	0.2541	0.00002	0.03172	0.009984

IV. Conclusion

Densities and viscosities of binary solutions of n-butyl acetate (1) and isopropanol (2) are measured at 305, 310, 315 and 320 K. Observed positive excess molar volumes assignable breaking of hydrogen bond of isopropanol molecule and negative Δη contribute to weak dipole-dipole interaction. Values of V_m^E and Δη have been fitted in Redlich-Kister polynomial equation. The results obtained revealed weak molecular interaction between solute-solvent molecules of binary solutions studied.

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