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Investigation of Specific Interactions between the Constituent Molecules of Binary Liquid Mixtures of Methyl benzoate, Ethyl benzoate and Benzyl benzoate with 2-Pentanol at Different Temperatures

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ABSTRACT

The current work focuses on the understanding of viscosity, density and ultrasonic velocity and their deviation of binary liquid mixtures of Methyl benzoate, Ethyl benzoate and Benzyl benzoate with 2 Pentanol at temperature 298.15K and 308.15K.The composition of liquid mixtures is taken in terms of mole fraction from 0.1 to 1.0. From these data, excess molar volume, deviation in viscosity and isentropic compressibility have been calculated. These calculated quantities have been utilized in Redlich-Kister equation to get the coefficients and standard errors. These parameters for the liquid mixtures have been adopted in the study of the molecular interactions and the effects of methyl, ethyl and benzyl group of benzoates present on benzene ring.

Keywords: Excess molar volume, Deviation in viscosity, Molecular interactions, Isentropic compressibility, Mole fraction.

INTRODUCTION

Molecular interactions in binary liquid mixtures have been playing a crucial role in laboratory research since long back[1-2]. 2-Pentanol is having many uses such as food additive, food additive flavour, antifreeze agent, cleaning agent, ion exchange agent, fuel, fuel additives, in industrial gas manufacturing and petroleum refineries. Methyl benzoate, ethyl benzoate and benzyl benzoate being polar solvents are utilized in many designing applications. Methyl and ethyl benzoate and benzyl benzoate have been broadly used in the flavouring, perfumery, artificial essences and cosmetics. Numerous works have been performed on the binary mixtures of above said esters recently[17-20] but no studies on properties such as density, viscosity and ultrasonic velocity for binary mixture of these esters with 2-pentanol have been accounted so far in literature survey. Calculations of density, viscosity and ultrasonic velocity could find broad applications in making characterization the thermodynamic and physico-chemical aspects of binary liquid mixtures as the constituent components have

wide applications in industry and other fields as disclosed earlier. The main intention of this study is to elaborate molecular interactions by using excess functions such as excess volume, deviation in viscosity and isentropic compressibility factor in the studied binary liquid mixtures.

MATERIALS AND METHODS

The solvent used was 2-Pentanol and imported from Sigma Germany having purity 99%. The solutes are Methyl benzoate, Ethyl benzoate, and Benzyl benzoate of Acros having purity 99% were utilized after first distillation. Experimental values of density, viscosity and ultrasonic velocities of pure liquids are compared at 298.15K, 303.15K, and these values are demonstrating acceptable concurrence with literature values published.[3-14] Specially designed stoppered bottles were used to prepare mixtures in terms of mole fractions. All the mixtures were utilized on same day for the estimations of above said parameters. Electronic balance of Adair Dutt with an accuracy of 0.0001 mg was used to prepare the binary mixtures. Digital densitometer model number DMA 35-84138 manufactured by Anton Par with an accuracy of 0.001 gm/cm^3, reproducibility of 0.0007 gm/cm^3 having capacity 2 mL, was used to measure the densities of pure liquids and their binary mixtures. Digital viscometer model number LVDVII+Pro manufactured by Brookfield Engineering Laboratories, Middleboro INC [USA], calibrated with triply distilled water with an accuracy ± 1% of full scale of range and viscosity repeatability ± 2% , was used to measure the viscosities of pure liquid and their binary liquid mixtures. Variable path single crystal interferometer from Mittal Enterprises F-05(SI No.1415071) model, New Delhi having frequency 2 MHz (with precision of ± 0.8 meter per second), was used to measure ultrasonic velocities of pure liquids and its binaries. Calibration of interferometer was done by using triply distilled water, methanol and benzene.

Table 1: Comparison of experimental and literature values of density, viscosity and ultrasonic velocity of 2-Pentanol, Methyl benzoate, Ethyl benzoate and Benzyl benzoate at 298.15K and 308.15K

Sr. No	Chemical	Temp/K	Density(gm.cm^{-3})		Viscosity(mPas)		Ultrasonic velocity(ms^{-1})	
			Expt	lit	Expt	lit	Expt	lit
1	2-Pentanol	298.15	0.8050	0.8054a,b,c	3.273	3.478a,b,,c	1232	1232j
		308.15	0.7984	0.7987c	2.494	2.370i	1197	-
2	Methyl benzoate	298.15	1.0832	1.0836d	1.819	1.825d	1406	1406d
		308.05	1.0736	1.0739e	1.503	1.510d	1370	1372e
3	Ethyl benzoate	298.15	1.0419	1.0413f	1.932	1.936e	1374	1378l
		308.15	1.0329	1.0325e	1.594	1.591e	1338	1338k
4	Benzyl benzoate	298.15	1.1226	-	8.287	8.292g	1530	-
		308.15	1.1139	1.1131h	5.226	5.229h	1482	1486h

References:-a= 3, b= 4,c= 5,d= 6,e= 7,f= 8,g= 9,h= 10, i= 11, j=12,k= 13,l=14

Table 2: Experimental values of density (ρ), viscosity (η), excess molar volume (V^E) deviations in viscosity (Δη), isentropic compressibility (ΔKs) for 2- Pentanol + Methyl benzoate

Temp/K	x_1	ρ x10^{-3} Kg.m^{-3}	ηmPa.s	Um/s	V^Ex10^{6}m^3.mol^{-1}	ΔηmPa.s	ΔKsTpa^{-1}
	0.0000	1.0832	1.819	1406	0.000	0.000	0.000
	0.0992	1.0562	1.655	1364	0.311	-0.308	7.200
	0.2009	1.0290	1.531	1330	0.502	-0.580	12.500
	0.2994	1.0025	1.404	1302	0.630	-0.850	15.900
	0.4002	0.9752	1.281	1279	0.701	-1.120	18.500
298.15K	0.5091	0.9454	1.169	1261	0.715	-1.390	20.300
	0.6007	0.9199	1.178	1249	0.693	-1.514	19.200
	0.6984	0.8924	1.304	1240	0.615	-1.530	16.900
	0.8003	0.8631	1.643	1234	0.502	-1.340	12.100
	0.8998	0.8342	2.222	1232	0.310	-0.905	7.200
	1.0000	0.8050	3.273	1232	0.0000	0.000	0.000
	0.0000	1.0736	1.503	1370	0.000	0.000	0.000
	0.0992	1.0460	1.310	1326	0.422	-0.291	10.000
	0.2009	1.0191	1.202	1289	0.616	-0.500	18.900
	0.2994	0.9931	1.075	1260	0.721	-0.725	25.100
	0.4002	0.9661	1.005	1237	0.794	-0.895	28.900
308.15K	0.5091	0.9365	0.949	1218	0.825	-1.059	31.000
	0.6007	0.9114	0.981	1207	0.789	-1.117	29.400
	0.6984	0.8841	1.073	1200	0.724	-1.122	25.000
	0.8003	0.8554	1.301	1196	0.572	-0.995	18.600
	0.8998	0.8269	1.737	1196	0.367	-0.658	9.900
	1.0000	0.7984	2.494	1197	0.000	0.000	0.0000

Table 3: Experimental values of density (ρ), viscosity (η), excess molar volume (V^E), deviations in viscosity (Δη) and isentropic compressibility (ΔKs) for 2- Pentanol + Ethyl benzoate

Temp/K	x_1	ρx10^{-3} Kg.m^{-3}	ηmPa.s	Um/s	V^Ex10^{6}m3.mol^{-1}	ΔηmPa.s	ΔKsTpa^{-1}
	0.0000	1.0419	1.932	1374	0.000	0.000	0.000
	0.0992	1.0214	1.738	1341	0.258	-0.329	5.300
	0.2009	1.0008	1.647	1312	0.437	-0.554	9.500
	0.2994	0.9794	1.531	1288	0.563	-0.805	13.400
	0.4002	0.9575	1.439	1269	0.632	-1.030	15.600
298.15K	0.5091	0.9352	1.345	1252	0.664	-1.255	16.400
	0.6007	0.9109	1.376	1243	0.650	-1.361	15.800
	0.6984	0.8861	1.487	1236	0.584	-1.384	13.800
	0.8003	0.8605	1.779	1232	0.468	-1.224	9.300
	0.8998	0.8331	2.357	1231	0.312	-0.781	5.100
	1.0000	0.8050	3.273	1232	0.0000	0.000	0.000
	0.0000	1.0329	1.594	1338	0.000	0.000	0.000
	0.0992	1.0121	1.423	1301	0.332	-0.262	9.000
	0.2009	0.9916	1.334	1271	0.528	-0.440	16.600
	0.2994	0.9705	1.255	1247	0.644	-0.610	22.100
	0.4002	0.9487	1.174	1227	0.731	-0.780	26.100
308.15K	0.5091	0.9267	1.142	1210	0.752	-0.900	30.200
	0.6007	0.9026	1.173	1202	0.745	-0.961	26.400
	0.6984	0.8781	1.255	1196	0.671	-0.969	21.900
	0.8003	0.8527	1.466	1194	0.562	-0.847	16.100
	0.8998	0.8258	1.821	1194	0.373	-0.582	9.000
	1.0000	0.7984	2.494	1197	0.000	0.000	0.000

Table 4: Experimental values of density (ρ), viscosity (η), excess molar volume (V^E), deviations in viscosity (Δη) and isentropic compressibility (ΔKs) for 2-Pentanol + Benzyl benzoate

Temp/K	x_1	ρx10^{-3} Kg.m^{-3}	ηmPa.s	Um/s	V^Ex10^{6}m^3.mol^{-1}	ΔηmPa.s	ΔKsTpa^{-1}
298.15K	0.0000	0.0000	8.287	1530	0.000	0.000	0.000
	0.0992	0.0986	7.434	1448	0.342	-0.359	9.400
	0.2009	0.1985	6.661	1384	0.523	-0.631	16.700
	0.2994	0.3009	5.865	1333	0.662	-0.913	20.900
	0.4002	0.3992	5.115	1296	0.725	-1.170	23.900
	0.5091	0.5000	4.365	1265	0.763	-1.415	24.800
	0.6007	0.5993	3.713	1244	0.756	-1.569	23.300
	0.6984	0.7004	3.185	1229	0.673	-1.590	20.100
	0.8003	0.7994	2.895	1222	0.547	-1.384	16.800
	0.8998	0.9006	2.807	1222	0.335	-0.964	9.500
	1.0000	1.0000	3.273	1232	0.000	0.000	0.000
308.15K	0.0000	1.1139	5.226	1482	0.000	0.000	0.000
	0.0992	1.0926	4.686	1399	0.417	-0.271	13.200
	0.2009	1.0705	4.182	1335	0.621	-0.502	23.200
	0.2994	1.0462	3.673	1285	0.751	-0.731	30.000
	0.4002	1.0209	3.181	1248	0.823	-0.954	34.000
	0.5091	0.9925	2.699	1220	0.857	-1.161	35.800
	0.6007	0.9618	2.292	1200	0.833	-1.297	34.200
	0.6984	0.9271	1.985	1188	0.768	-1.328	30.100
	0.8003	0.8894	1.854	1182	0.618	-1.188	23.600
	0.8998	0.8460	2.000	1185	0.403	-0.766	13.600
	1.0000	0.7984	2.494	1197	0.000	0.000	0.000

Table 5: Parameters of Jouyban-Acree model and average percentage deviation for density, viscosity and ultrasonic velocity for the binary systems

System- 2 Pentanol +	A_0	A_1	A_2	A_3	A_4	APD
			Density			
Methyl benzoate	17.8036	3.5778	-3.9143	-	-	0.0112
Ethyl benzoate	24.5139	4.8573	-1.9546	-	-	0.0063
Benzyl benzoate	62.7306	21.9791	6.3680	2.8598	-1.7017	0.0086
			Viscosity			
Methyl benzoate	-856.4083	-481.0626	133.2435	295.5697	-166.3345	0.7869
Ethyl benzoate	-695.6763	-395.7238	41.3756	244.2325	-115.0130	0.7600
Benzyl benzoate	-294.4104	-531.1567	-399.2081	2.7034	85.9469	1.3772
			Ultrasonic Velocity			
Methyl benzoate	-57.8511	8.6331	-0.6037	1.7135	3.4310	0.1118
Ethyl benzoate	-51.4108	4.9804	6.9962	0.7109	-5.4495	0.1049
Benzyl benzoate	-106.5277	11.1042	-13.4274	2.1571	-	0.1324

Table 6: Interaction parameters for the binary system

System- 2-Pentanol +	Temp/K	d	σ	W_{visc}/RT(kj.mol^{-1})	σ	H_{12}mPa.s	σ
Methyl benzoate	298.15	-2.809	0.13	-2.933	0.14	-0.344	0.220
	308.15	-2.788	0.06	-2.739	0.06	-0.232	0.110
Ethyl benzoate	298.15	-2.427	0.10	-2.503	0.11	-0.037	0.170
	308.15	-2.229	0.05	-2.156	0.05	0.122	0.090
Benzyl benzoate	298.15	-0.918	0.13	-0.914	0.14	2.747	0.100
	308.15	-1.395	0.11	-1.213	0.10	1.370	0.080

Where d, W_{visc}, H_{12} are the interaction parameters and σ is the standard deviations

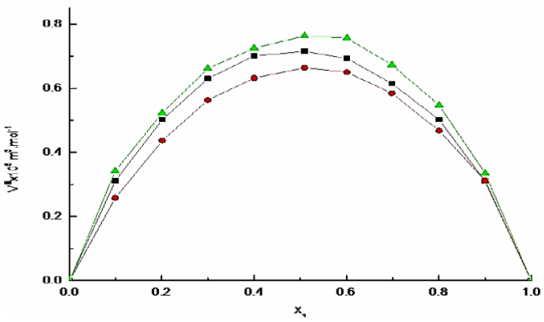

Fig. 1. Plot of excess molar volume against mole fraction of 2-pentanol (x1) with (1-x1) mole fractions of methyl benzoate (□), ethyl benzoate (•) and benzyl benzoate (Δ) at 298.15K

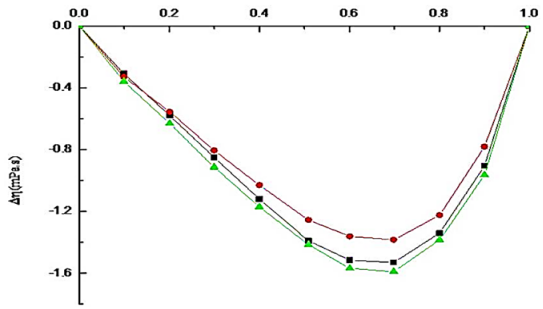

Fig. 2. Plot of deviation in viscosity against mole fraction of 2-pentanol (x1) with (1-x1) mole fractions of methyl benzoate(□), ethyl benzoate (•) and benzyl benzoate(Δ) at 298.15K

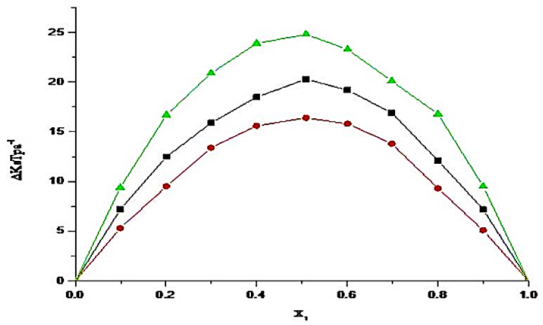

Fig. 3. Plot of deviation in compressibility factor against mole fraction of 2-pentanol (x1) with (1-x1) mole fractions of methyl benzoate (□), ethyl benzoate(•) and benzyl benzoate (Δ) at 298.15K

RESULT AND DISCUSSION

The values of density, viscosity and ultrasonic velocity as a function of mole fractions obtained from an experiment at temperature 298.15 and 308.15K are clearly tabulated. The values of density are exercised to compute the excess molar volumes VE by employing the equation,

$$V^E/(cm^3.mole^{-1}) = (x_1M_1+x_2M_2)/\rho_{12}-(x_1M_1/\rho_1) - (x_2M_2/\rho_2) \quad (1)$$

Where ρ_{12} is the density of the mixture, x_1, M_1, ρ_1 and x_2, M_2, ρ_2 are the mole fractions, molecular weights and densities of pure components 1 and 2 respectively.

The deviations in viscosities $\Delta\eta$ were estimated by employing the relation,

$$\Delta\eta = \eta_{12} - x_1\eta_1 - x_2\eta_2 \quad (2)$$

Where η_{12} is the viscosity of the mixture, x_1, x_2 and η_1, η_2 are the mole fractions and viscosities of the pure components 1 and 2 respectively.

The excess isentropic compressibilities (Ks) were computated by employing the relation,

$$Ks = 1/u^2p \quad (3)$$

Where u is the ultrasonic velocity p is the density.

And the deviation in isentropic compressibilitis (ΔKs) were estimated by using the relation,

$$\Delta Ks = Ks_{(12)} - x_1 Ks_1 - x_2 Ks_2 \quad (4)$$

Where $Ks_{(12)}$ is the compressibilities of the

mixture, x_1, x_2 and, Ks_1, Ks_2 are the mole fractions and isentropic compressebilities of the pure components 1 and 2 respectively.

The excess molar volumes, deviation in viscosities and isentropic compressibilitis were put into Redlich Kister equation of following type,

$$Y=x_1 x_2 \sum_i^n \alpha_i (x_1-x_2)^i \quad (5)$$

Where Y is either, V^E, $\Delta\eta$, or ΔKs and n is the degree of polynomial. Coefficients ai were sought by applying equation 5 to experimental results using a least-squares regression method. In each case, the numbers of coefficients are determined from the examination of variation in standard deviation (σ) and it was estimated by adopting the equation,

$$\sigma(Y) = [\sum (Y_{expt}- Y_{cal})^2]^{1/2}/ N-n \quad (6)$$

Where N is the number of data points and n is the number of coefficients. The computated values of the coefficients (a_i) along with the standard deviations (σ) are displayed in the Table 6.

Hind *et al.,* offered an equation for the viscosity of binary liquid mixtures as,

$$\eta = x^1_2.\ln\eta_1+ x^1_2.\ln\eta_2 + 2x_1x_2 H_{12} \quad (7)$$

Where x_1, x_2, η_1, η_2 are the mole fractions and viscosities of solvent and solute respectively and H_{12} is the interaction parameter.

Katti and Chaudhari suggested following equation.

$$\log (\eta mVm) = x_1\log(\eta_1V_1) + x_2\log(\eta_2V_2) + x_1x_2[Wvis/(RT)] \quad (8)$$

Where η_m and V_m are the viscosity and volume of the mixture, Wvis is defined as interaction energy for the activation of flow.

The Jouyban and Acree proposed a model for correlating the density and viscosity of liquid mixtures at various temperatures. The equation is,

$$\ln y_{m,T}= f_1 \ln y_{1,T} + f_2 \ln y_{2,T} + f_1f_2 \sum[A_j (f_1-f_2)j /T] \quad (9)$$

Where $y_{m,T}$, y_1, T and $y_{2,T}$ is density or viscosity of the mixture and solvent 1 and 2 respectively at given temperature T and f_1, f_2 are the mole fractions and A_j are model constants.

Jouyban–Acree model is applied to the density, viscosity and speed of sound of data and the correlating ability of this model was tested by calculating the average percent deviation (APD) between the experimental and calculated density, viscosity and speed of sound as

$$APD = (100/N) \sum [(y_{expt}–y_{calc})/y_{expt}] \quad (10)$$

Where N is the number of data points in each set, y represents density or viscosity. The optimum number of constants A_j and in each case they were determined from the examination of APD values.

Density, viscosity, ultrasonic velocity, deviation in viscosity, excess volume and compressibility factor for binary liquid mixtures containing 2-pentanol with methyl benzoate, ethyl benzoate and benzyl benzoate at 298.15K and 308.15K have been computed over entire range of composition of mole fractions and shown in table 2,3 and 4. Parameters of Jouyban-Acree model and average percentage deviation for density, viscosity and ultrasonic velocity are also disclosed in Table 5 while interaction parameters for the binary system in Table 6.

The excess volume variation (disparity) with mole fraction x_1 of 2-Pentanol with methyl benzoate, ethyl benzoate and benzyl benzoate at 398.15K is clearly shown in Fig. 1. Literature[15-18] gives excess volume variation of methyl benzoate and ethyl benzoate with alcohols at 298.15K but no data have been reported so far for methyl benzoate and ethyl benzoate with 2-pentanol. It has been observed from the data and graphical representation that excess volume and deviation in compressibility factor show positive deviation with maxima at mole fraction 0.5 for 2-Pentanol with methyl benzoate, ethyl benzoate and benzyl benzoate system over entire range of composition of mole fraction in figure 1 and 3 whereas deviation in viscosity for all systems are showing negative deviation with minima at mole fraction 0.7 depicted in Fig. 2 and it has been observed that $\Delta\eta$ are negative for all systems showing the weak interactions present in the binary mixtures under consideration. $\Delta\eta$ values slightly increase with increase in temperature,[19]

and are negative for all systems showing the weak interactions present in the binary mixtures and the credit of such behaviour goes to breaking of dipole-dipole interaction as well as interactions formation between the polar benzoate group and electron donating methyl, ethyl and benzyl group. The trend of excess volume is, 2-pentanol + benzyl benzoate > 2-pentanol + methyl benzoate > 2 -pentanol + ethyl benzoate. It has been also shown that excess volume increases with increase in temperature for all three binary systems.

CONCLUSION

Calculations of excess volume, deviation in viscosity and deviation in compressibility factor derived from density, viscosity and ultrasonic velocity are clearly indicating the weak interactions are present in binary liquid mixtures at specific composition. The knowledge of these interactions could be used in many industrial applications.

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Conflict of interest

The authors declare no conflict of interest.

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