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Investigation Of Thermophysical Properties Of Acetophenone And Ethyl 2-Methyl Butyrate Binary Mixtures At Different Temperatures.

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ABSTRACT

In this article the behavior of Acetophenone and Ethyl 2-Methyl Butyrate binary mixtures have been investigated with the temperature varying from 303.15–323.15 K as a function of composition through the measurement of viscosity and density. From these data, molar volume, deviations in viscosity, refractive index deviation have been calculated. These results are fit to the Redlich-Kister polynomial to derive the binary coefficients and the standard error values are also estimated. The calculated parameter values and their deviations of the liquid binary mixture indicate a particular type of interaction between the unlike molecules.
Keywords: Molecular Interactions; Viscosity; Density; Excess Volume; Viscosity Deviation

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INTRODUCTION

Non ideal solutions are distinguished by defining the strength of the intermolecular forces among different molecules in that specific solution [1]. Studies in solution theory and molecular dynamics requires the data on some of the thermophysical properties associated with the liquids and liquid mixtures. These findings made it obvious to study the density and viscosity of liquid mixtures and their dependence with composition and temperature. In the recent years, the need for the thermophysical properties are raising and it is very significant in different applications, like design of distillation columns, pipeline systems and mass transfer operations [2]. Liquid mixtures have attracted extensive attention because of their unusual behaviour. Studies on determination of various thermophysical properties of liquid mixtures within wide range of temperature and composition are important source of information which can be used to study the relation between physical properties and the internal structure of the system. The deviations from ideality of binary mixtures are arised not only from difference in size of the molecule but due to structural changes also [3].

Acetophenone is an essential chemical used in industries broadly as an ingredient of flavor and aroma in soaps, cleansers, cosmetics and perfumes. It is also widely used in pharmaceutical and agrochemicals as an important intermediate. Ethyl-2-Methylbutyrate is significant ester in industries related to flavor and fragrance manufacturing process [4]. The deviation values have been fitted to Redlich-Kister type equations [5].To our knowledge the density and viscosity of Ethyl-2-Methylbutyrate in binary mixtures with Acetophenone at various temperature and composition have not been examined.

MATERIALS AND METHODS

All the chemicals used in this work were supplied by Loba chemicals (purity ≈ 99%). Digital electronic balance with an accuracy of ±0.0001 g (Mettler-AE 240, Switzerland) was used to measure the weight of the empty bottle and airtight stoppered bottles (to prevent evaporation) were used to prepare the binary mixtures [6]. A double armed pycnometer was used to measure the density values of liquid and liquid mixtures. Pycnometer was calibrated using freshly prepared triple distilled water. A digital electronic balance was used in the density measurements. Ostwald's viscometer was used to measure the viscosity values of pure and binary liquid mixtures and calibrated using double distilled water [7-10]. The time flow was measured using a digital stop watch (19671697- Edutek, India) with an accuracy of ±0.01 s.

RESULTS AND DISCUSSIONS

The purity of chemical were checked by comparing their densities and viscosities with literature values and presented in table 1. The values observed from table 1 shows the experimental values are fairly well with the literature values. The experimental densities ρ and viscosities η for studied binary mixtures at 303.15 -323.15 K are given in Table 2.

The calculated values like excess molar volume, deviation of viscosity, and refractive index deviation were computed from the experimental data according to the following relations

$$V^E = \sum_{i=1}^{n} x_i \, M_i(\rho^{-1} - \rho_i^{-1}) \quad (1)$$

$$\eta^E = \eta - \sum_{i=1}^{n} x_i \, \eta_i \quad (2)$$

$$\Delta n_D = n_D - \sum_{i=1}^{n} x_i \, n_{Di} \quad (3)$$

where x_i represent the mole fraction of the pure component i. M, ρ, η and n_D are the molar volume, density, viscosity and refractive index of pure components respectively. M_i, ρ_i, η_i and n_{Di} are the corresponding properties of the binary mixtures of components. The calculated excess property values such as V^E, $\Delta\eta$ and Δn_D of binary liquid mixtures are shown in Table 3.

The calculated values of excess properties such as excess molar volume, deviation of viscosity, and excess refractive index deviation are fitted with Redlich–Kister polynomial equation[Redlich and Kister, 194],

$$A^E = x_1(1-x_1) - \sum_{i=1}^{n} A_i(2x_2-1)^i \quad (4)$$

Method of least square fit was used to calculate the values of A_i in Eq. (4). The standard deviation of the experimental and theoretical values are identified from the parameter values of each studied system. The standard deviation values are summarized by the following relation,

$$\sigma = \left[\frac{\sum(x_{exp}-x_{calc})^2}{n-p}\right]^{1/2} \quad (5)$$

where n is the number of experimental points, p is the number of parameters, x_{exp} and x_{cal} are the experimental and calculated properties. The calculated values of coefficients along with standard deviation (σ) are given in Table 4.

The plots representing deviation in viscosity at 303.15, 313.15 and 323.15 K against mole fraction for binary mixtures of Acetophenone with ethyl 2- methyl butyrate are presented in Fig 1. Deviation in viscosity values (Negative deviation) specify that the dominant forces are dispersion forces [12-14]. Deviation increases with increase in temperature which shows the forces between different (unlike) molecules are lesser compared to the forces between like molecules. It also suggests the existence of weak intermolecular interactions when mixing occurs in ethyl 2–methyl butyrate. Excess molar volumes of mixtures against mole fraction at 303.15, 313.15 and 323.15 K for binary mixtures of acetophenone with ethyl 2- methyl butyrate are represented in fig 2. These plots specify that the V^E are positive for all studied temperatures and increases with temperature [15].The excess molar volume value signifies the several opposing effects in liquid mixture. Positive term to excess molar volume V^E is due to the contribution of a nonspecific interaction between the real species existing in the mixture [16, 17]. The plots representing deviation in refractive index at 303.15, 313.15 and 323.15 K against mole fraction for liquid mixtures of Acetophenone with ethyl 2- methyl butyrate are presented in Fig 3. Deviation in refractive index values (Negative deviation) over the entire range of composition signifies that the size and shape of the molecules plays an important role along with the strength of specific interaction.

Table 1: Experimental values (density and viscosity) of pure liquids compared with literature values at 303.15 – 323.15 K

Temp	Density ρ (gcm^{-3})		Viscosity η (mPa·s)		Refractive index	
	Exp	Literature	Exp	Literature	Exp	Literature
Acetophenone						
303.15	1.0198	1.0199 [10,11]	1.5431	1.5400 [10,11]	1.5221	1.5221 [10,11]
313.15	1.0109	1.0110 [10,11]	1.3173	1.3175 [10,11]	1.5171	1.5172 [10,11]
323.15	0.9987	0.9987 [10,11]	1.2853	1.2855 [10,11]	1.5043	1.5041 [10,11]
Ethyl 2-Methyl Butyrate						
303.15	0.8614	0.86148 [4]	0.72310	0.723 [4]	1.3868	
313.15	0.8534	0.85341 [4]	0.6351	0.635 [4]	1.3561	
323.15	0.8467		0.56305		1.3121	

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Table 2: Experimental values (Density, viscosity and refractive indices) for binary mixtures at specified temperatures (303.15 – 323.15 K)

x	ρ (gcm-3)	η (mPa.s)	nD	ρ (gcm-3)	η (mPa.s)	nD	ρ (gcm-3)	η (mPa.s)	nD
	303.15 K			313.15 K			323.15 K		
0	0.8615	0.7231	1.3868	0.8534	0.7231	1.3561	0.8467	0.5631	1.3121
0.1250	0.8773	0.7961	1.4003	0.8691	0.7741	1.3722	0.8619	0.6128	1.3315
0.2432	0.8932	0.8692	1.4139	0.8849	0.8251	1.3883	0.8772	0.6626	1.3509
0.3552	0.9089	0.9422	1.4274	0.9006	0.8760	1.4044	0.8924	0.7124	1.3703
0.4615	0.9248	1.0152	1.4409	0.9163	0.9270	1.4205	0.9075	0.7622	1.3897
0.5625	0.9407	1.0882	1.4545	0.9320	0.9780	1.4366	0.9227	0.8119	1.4091
0.6585	0.9565	1.1613	1.4679	0.9477	1.0289	1.4527	0.9379	0.8618	1.4285
0.7502	0.9723	1.2343	1.4815	0.9635	1.0799	1.4688	0.9531	0.9116	1.4479
0.8372	0.9882	1.3073	1.4950	0.9792	1.1309	1.4849	0.9683	0.9614	1.4673
0.9204	1.0040	1.3803	1.5086	0.9949	1.1819	1.5011	0.9835	1.0111	1.4867
1	1.0198	1.5431	1.5221	1.0109	1.3173	1.5171	0.9987	1.2853	1.5043

Table 3: Excess molar volume V^E, deviation of viscosity Δη, and deviation of refractive index Δn_D, for binary mixtures at specified temperatures (303.15- 323.15 K)

x_1	Δη mPa.s	V^E cm^3/mol	Δn_D	Δ η mPa.s	V^E cm^3/mol	Δn_D	Δ η mPa.s	V^E cm^3/mol	Δn_D
	303.15 K			313.15 K			323.15 K		
0	0	0	0	0	0	0	0	0	0
0.1250	-0.0173	0.0058	-0.0034	-0.0148	0.0072	-0.0040	-0.0125	0.0093	-0.0049
0.2432	-0.0286	0.0099	-0.0059	-0.0241	0.0128	-0.0069	-0.0215	0.0153	-0.0084
0.3552	-0.0354	0.0125	-0.0075	-0.0302	0.0158	-0.0089	-0.0275	0.0185	-0.0107
0.4615	-0.0379	0.0136	-0.0083	-0.0334	0.0172	-0.0099	-0.0306	0.0199	-0.0119
0.5625	-0.0387	0.0136	-0.0085	-0.0339	0.0171	-0.0101	-0.0311	0.0199	-0.0121
0.6585	-0.0368	0.0125	-0.0079	-0.0319	0.0161	-0.0094	-0.0292	0.0188	-0.0114
0.7502	-0.0325	0.0105	-0.0068	-0.0275	0.0138	-0.0081	-0.0249	0.0167	-0.0097
0.8372	-0.0252	0.0077	-0.0050	-0.0209	0.0099	-0.0060	-0.0185	0.0131	-0.0072
0.9204	-0.0139	0.0042	-0.0028	-0.0124	0.0057	-0.0033	-0.0102	0.0082	-0.0039
1	0	0	0	0	0	0	0	0	0

Table 4: Values of adjustable parameters (A_k) and the Corresponding Standard Deviation (σ) for deviation of viscosity (Δη), excess molar volumes (V^E), and deviation of refractive index Δn_D for binary liquid mixtures at 303.15 - 323.15 K

Parameter/ Function	T/K	A_0	A_1	A_2	A_3	A_4	σ
Acetophenone (1) + Ethyl 2-Methyl Butyrate (2)							
Δη (mPa.s)	303.15	-0.151	-0.0582	-0.3235	0.0409	0.4609	0.0005
	313.15	-0.1313	-0.0511	-0.2646	0.0352	0.3828	0.0002
	323.15	-0.1233	-0.049	-0.1985	0.0367	0.312	0.0007
V^E (cm^3/mol)	303.15	0.0551	0.0137	0.0825	-0.0091	-0.1335	0.0003
	313.15	0.0683	0.0191	0.1168	-0.0119	-0.1796	0.0002
	323.15	0.077	0.027	0.1864	-0.0156	-0.2544	0.0006
Δn_D	303.15	-0.0335	-0.0133	-0.0539	0.01	0.0848	0.0003
	313.15	-0.0399	-0.0159	-0.0642	0.0119	0.1009	0.0002
	323.15	-0.048	-0.0191	-0.0774	0.0143	0.121	0.0005

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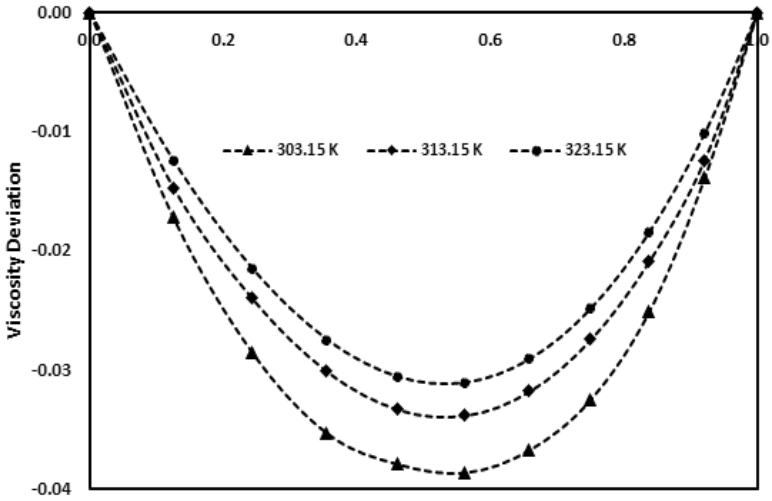

Fig.1. Plot of viscosity deviation Δη against mole fraction *x* of Acetophenone (1) + Ethyl 2-Methyl Butyrate (2)

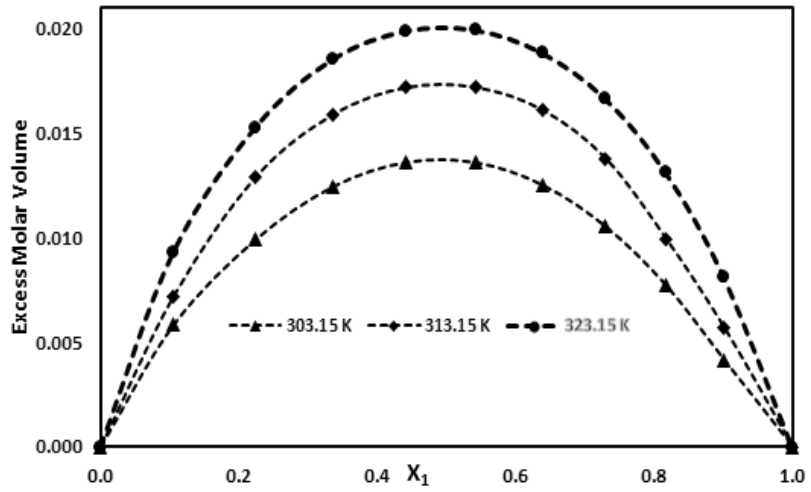

Fig.2. Plot of excess molar volume V^E against mole fraction *x* of Acetophenone (1) + Ethyl 2-Methyl Butyrate (2)

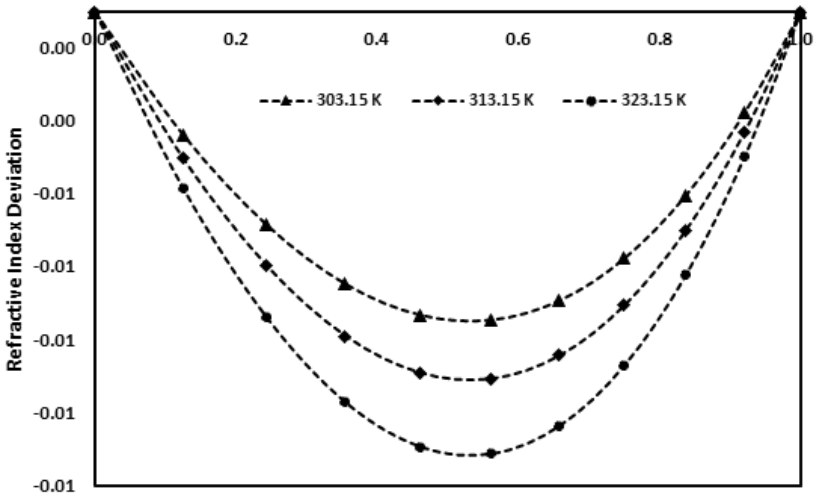

Fig.3. Plot of refractive index deviation Δn_D against mole fraction x of Acetophenone (1) + Ethyl 2-Methyl Butyrate (2)

CONCLUSION

Densities and viscosities for liquid mixtures have been measured. The pure component values mostly correspond to the existing literature values. Excess molar volumes, deviations of viscosity and refractive index of acetophenone and ethyl 2- methyl butyrate were obtained through the experimental results. The obtained results are fitted to the Redlich Kister equation and analysed in terms of interactions between the components at molecular level. Deviations of viscosity and refractive index, excess molar volumes of Acetophenone and ethyl 2- methyl butyrate at different temperatures has been reported. There is intermolecular interaction among the components of the binary mixture.

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