Refractive Indices and Surface Tension of Diacetone Alcohol + Benzene or Chlorobenzene at 303.15, 313.15 K and 323.15 K

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Abstract: The studies of refractive indices and surface tension are being increasingly used as tools for investigation of the properties of pure components and the nature of intermolecular interactions between the liquid mixture constituents. Refractive indices (n_D), and surface tension (σ) have been measured for the binary liquid mixture of diacetone alcohol + Benzene and diacetone alcohol +chlorobenzene over the entire composition range at 303.15, 313.15 K and 323.15 K. The Redlich-Kister model was used to correlate the measured properties. It was found that in all cases, the experimental data obtained fitted with the values correlated by the corresponding models very well. The molecular interactions existing between the components were also discussed.

Keywords: Diacetone alcohol; refractive indices; surface tension

1. Introduction

Binary liquid mixtures due to their unusual behavior have attracted considerable attention [1]. Data on some of the properties associated with the liquids and liquid mixtures like refractive index, ultrasonic velocities and surface tension find extensive application in chemical engineering process simulation, solution theory and molecular dynamics [2]. These properties are important from practical and theoretical point of view to understand liquid theory. These mixtures are used in the titration calorimetry and reaction calorimetry. We have reported refractive index and surface tension of pure diacetone alcohol + benzene and diacetone alcohol + chlorobenzene at temperatures of 303.15, 313.15 K and 323.15 K.

The values have been fitted to Redlich-Kister type [3] equation. Literature survey showed that no measurements have been previously reported for the mixture studied in this paper.

2. Material and Methods

The chemicals used were of analytical grade and obtained from lobo chemicals. All the components were dried over anhydrous potassium carbonate and fractionally distilled [4]. A thermostatically controlled well-stirred water bath whose temperature was controlled to ±0.01 K accuracy was used for all the measurements. All the measurements were done by using electronic balance Shimadzu Corporation Japan Type BL 2205 accurate to

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0.01 g. The possible uncertainty in the mole fraction was estimated to be less than ±0.0001.

2.1. Refractive indices

Refractive indices were measured using thermostatically controlled Abbe refractometer (Atago 3T) with accuracy less than 0.0001units.A minimum of three independent readings were taken for each composition and the average value was considered in all the calculations. Water was circulated in to the prism of the refractometer by a circulation pump connected to an external thermostated water bath. Calibration was performed by measuring the refractive indices of doubly distilled water and propyl alcohol at defined temperatures. The sample mixture was directly injected in to the prism assembly of the instrument using a syringe. The solutions were pre thermostated at the temperature of the experience before the experiments to achieve a quick thermal equilibrium. The change of refractive index over the composition range was obtained by

$$\Delta n_D = n_{D} - (x_1 n_{D1} + x_2 n_{D2}) \qquad (1)$$

Where n_D is the refractive index of the mixture and n_{D1} and n_{D2} are the refractive indices of the pure compounds.

2.2. Surface tension

Surface tension was determined using drop volume tensiometer described in detail [5] which also discussed procedure and handling of data. The precision capillary is connected to a dosing system. It is located in one of the two liquid phases involved and forces the second liquid phase in to first liquid phase through the capillary. From the flow rate and number of drops, surface tension of each drop is calculated for pure liquid and the binary mixture over the whole composition range. All the samples were equilibrated to 313.15 K under atmospheric pressure. It was calibrated with distilled water. The accuracy of the surface tension measurement was estimated to be

0.1mNm$^{-1.}$ This can be calculated as

$$\sigma = V_{drop} (\rho_H - \rho_L) g / \pi d \qquad (5)$$

σ = Surface tension, V= Volume of drop, d=Dia of capillary, g = Acceleration, due to gravity.

3. Results and discussion

Table 1 summarizes the comparison of density, refractive index and surface tension data for liquids with literature. Table 2 lists the measured, refractive indices (n_D) and surface tension (σ) for the binary liquid mixture of Diacetone alcohol-benzene over the entire composition range at 303.15, 313.15 K and 323.15 K. Table 3 lists the measured, refractive indices (n_D) and surface tension (σ) for the binary liquid mixture of Diacetone alcohol- chlorobenzene benzene over the entire composition range at 303.15, 313.15 K and 323.15 K. A detailed observation of the Table 2 and 3shows that the surface tension of the mixture decreases with the mole fraction and temperature. According to Karla Granados [6] strong interaction in the liquid mixture decreases the σ value of the mixture. This means that interactions in the mixture are not strong and hence rise in the σ value was observed when mole fraction increases. It has also been observed that the refractive index deviation shows positive values for the entire mole fraction. It may be noted that such values are due to the electronic perturbation of the individual molecules during mixing and therefore depend very much on the nature of the mixing molecules [7]. It can be summarized that excess values may be affected by three factors. The first factor is the specific forces between molecules, such as hydrogen bonds, charge transfer complexes, breaking of hydrogen bonds and complexes bringing negative excess values [8]. The second factor is the physical intermolecular forces, including electrostatic forces between charged particles and between a permanent dipole and so on induction forces between a permanent dipole and an induced dipole and forces of attraction

and repulsion between non polar molecules. Physical intermolecular forces are weak and the sign of excess value may be positive and negative. Third factor is the structural characteristics of the component arising from geometrical fitting of one component in to other structure due to the differences in shape and size of the components and free volume. Our study shows that diacetone alcohol- benzene and diacetone alcohol – chlorobenzene system follows the above mentioned second factor and hence physical intermolecular forces are weak and the sign of excess values are positive or negative. In the present investigation the behavior of these systems has been interpreted qualitatively. In this binary mixture, it is assumed that on addition of benzene or chlorobenzene to diacetone alcohol, molecules may break in to several dipoles which in turn may induce dipole moment in the neighboring aromatic hydrocarbons forming the molecular association.

4. Conclusion

Experimental data of the density, refractive index, and surface tension of diacetone alcohol + benzene and diacetone alcohol + chlorobenzene mixture have been measured at 303.15, 313.15 K and 323.15 K. These data have been used to compute the excess properties of the system. The intermolecular interactions between diacetone alcohol + benzene and diacetone alcohol + chlorobenzene mixture leads to weak dispersive type. It is clear that Redlich kister polynomial equation can represent the deviations of refractive index and surface tension are very well by standard deviation values.

Table 1. Comparision of density, refractive index and surface tension data for liquids at 303.15K with the literature.

Pure liquids	ρ / g/cc		n_D		σ/ m.N.m^{-1}	
	Exp.	Lit	Exp.	Lit.	Exp.	Lit.
Diacetone alcohol	0.9360	0.9360	1.4230	1.4239[a]	28.12	29.44 [a]
Benzene	0.8450	0.8750[b]	1.4821	1.5000[c]	20.20	20.22 [c]
Chlorobenzene	1.1020	1.1020 [d]	1.5590	1.5590 [d]	33.60[d]	33.60[d]

[a]ref 9   [b] ref10 [c] ref 11 [c] ref 12[d]

Table 2. Experimental refractive indices (n_D) and surface tension (σ) of diacetone alcohol – benzene mixture at 303.15, 313.15 K and 323.15 K.

X_1	n_D	σ/m.N.m^{-1}	n_D	σ/m.N.m^{-1}	n_D	σ/m.N.m^{-1}
	303.15 K		313.15 K		323.15 K	
0.0000	1.5000	30.22	1.4821	20.20	1.4691	16.21
0.1225	1.4908	30.14	1.4755	21.29	1.4636	17.71
0.2525	1.4810	30.05	1.4680	22.44	1.4580	19.25
0.3224	1.4780	30.00	1.4651	23.05	1.4550	20.09
0.4218	1.4682	29.94	1.4590	23.93	1.4511	21.29
0.5045	1.4620	29.88	1.4540	24.66	1.4460	22.28
0.6112	1.4539	29.80	1.4470	25.61	1.4421	23.56
0.7123	1.4461	29.70	1.4401	26.47	1.4364	24.76
0.8191	1.4379	29.61	1.4330	27.39	1.4280	26.00
0.9337	1.4291	29.51	1.4250	28.37	1.4211	27.36
0.9337	1.4291	29.44	1.4198	28.92	1.4151	28.12

Table 3. Experimental refractive indices (n_D), surface tension (σ) of diacetone alcohol – Chlorobenzene mixture at 303.15, 313.15 K and 323.15 K.

X_1	n_D	$\sigma/m.N.m^{-1}$	n_D	$\sigma/m.N.m^{-1}$	n_D	$\sigma/m.N.m^{-1}$
	303.15 K		313.15 K		323.15 K	
0.0000	1.5590	33.60	1.5509	32.30	1.5480	31.26
0.1268	1.5440	33.50	1.5370	31.90	1.5335	30.99
0.2462	1.5285	33.01	1.5216	31.40	1.5185	30.51
0.3454	1.5160	33.00	1.5095	31.30	1.5070	30.40
0.4991	1.4950	32.50	1.4899	30.90	1.4866	30.00
0.5214	1.4910	31.80	1.4860	30.40	1.4840	29.41
0.6119	1.4785	31.60	1.4730	29.71	1.1730	28.81
0.7214	1.4630	31.20	1.4585	29.42	1.4581	28.56
0.8585	1.4443	30.71	1.4405	29.10	1.4360	28.32
0.9141	1.4365	30.11	1.4330	28.98	1.4285	28.24
1.0000	1.4239	29.44	1.4198	28.92	1.4151	28.12

Table 4. Redlich- kister Parameters and standard deviation of diacetone alcohol with benzene and diacetone alcohol with chloro benzene mixtures at T=(303.15,313.15 and 323.15) K

	Functions	303.15 K				313.15 K				323.15 K			
		A_0	A_1	A_2	S%	A_0	A_1	A_2	S%	A_0	A_1	A_2	S%
Diacetone alcohol + benzene	Δn_D	0.00	0.01	0.00	2.11	0.00	0.00	0.00	1.11	0.01	0.01	0.00	0.94
	$\Delta \sigma$	0.00	0.00	0.00	1.68	0.59	0.20	0.20	2.14	0.19	0.14	0.32	0.95
Diacetone alcohol + chloro benzene	Δn_D	0.06	0.02	0.002	1.98	0.07	0.02	0.003	1.42	0.01	0.018	0.00	0.89
	$\Delta \sigma$	0.44	2.45	-0.19	0.41	0.07	2.55	0.031	1.82	0.54	0.377	0.23	1.25
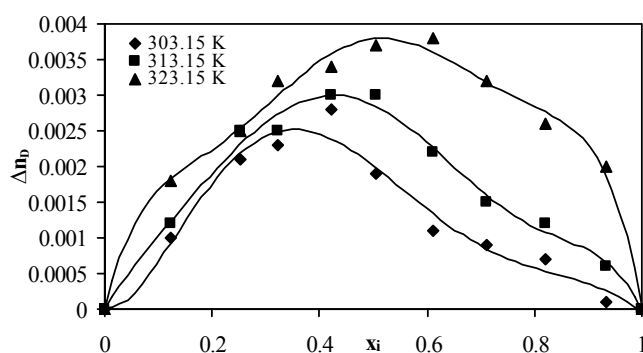
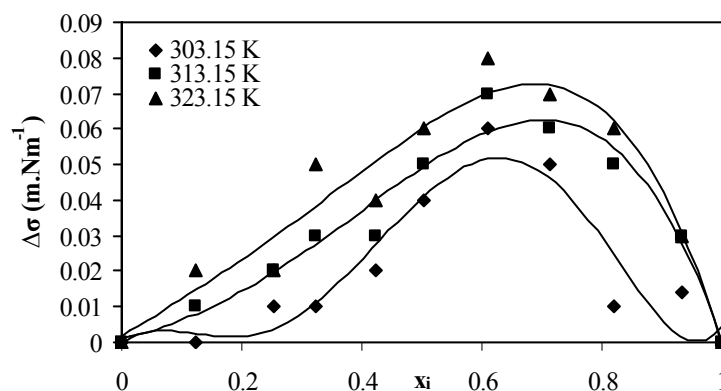Figure1. Deviations in refractive index (ΔnD) for diacetone alcohol and benzene at (303.15, 313.15 K, 323.15) K

Figure2. Deviations in surface tension (Δσ) for diacetone alcohol and benzene at (303.15, 313.15 K, 323.15) K
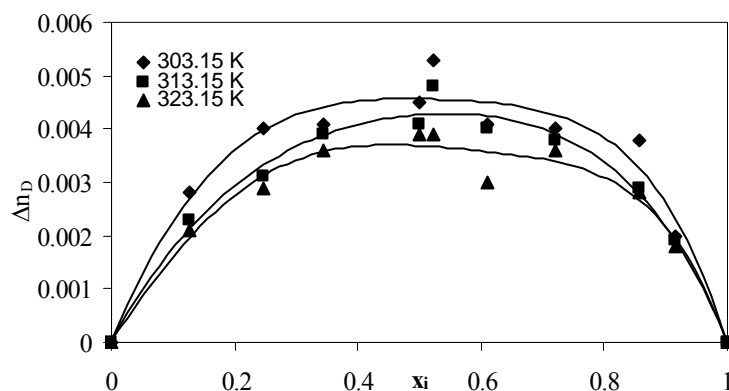

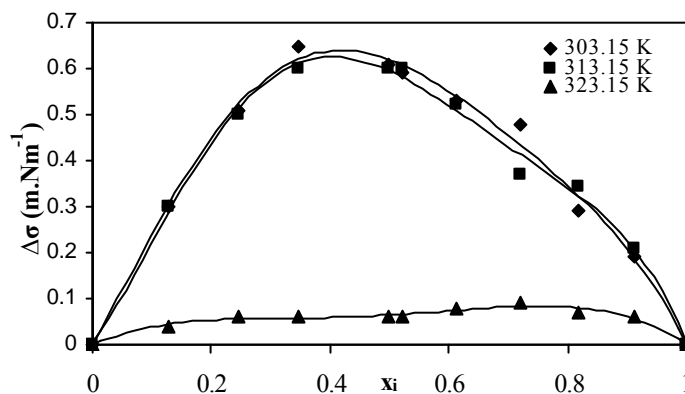Figure 3. Deviations in refractive index (ΔnD) for diacetone alcohol and chlorobenzene at (303.15, 313.15 K, 323.15) K

Figure 4. Deviations in surface tension (Δσ) for diacetone alcohol and chlorobenzene at (303.15, 313.15 K, 323.15) K

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