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Study of Excess Molar Volumes of the Binary Mixture of 1-Hexanol and Benzene at 303.15 K Temperature

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Abstract

The densities, ρ of pure 1-Hexanol, Benzene and their binary mixture covering the whole composition range have been measured at 303.15 K temperature. Excess molar volumes V_m^E, partial molar volumes, V_i have been calculated from the ρ data. To obtain correlation coefficients and standard deviations V_m^E was fitted to Redlich–Kister type function in terms of mole fraction. In the whole range of composition the values of V_m^E were found to be positive. The positive values of V_m^E were shown due to depolymerization of the network structures and disrupt their H-bonding and resulting into volume expansion.

Keywords: Density, Depolymerization, H-bonding, Molar volumes.

INTRODUCTION

The measurement of density, molar volume and related excess properties are included in the investigation of the physico-chemical behavior of liquid systems and provides useful information regarding the intermolecular interactions in liquids and their mixtures. This experimental data is useful for industrial objectives, for theoretical and applied thermodynamics. The nature and strength of molecular interactions can be known by studying the variation of thermo physical properties with several parameters which enables to determine the deviation and excess properties of mixtures [1-3]. In general, thermodynamic and transport properties are adequately employed in understanding the nature of molecular systems and physico- chemical behavior of liquid-liquid mixtures. In recent years several studies for alcohol + hydrocarbon [4-7] have been made on these properties of binary liquid mixtures in addition to their volumetric properties. Due to the presence of both hydrophilic and hydrophobic groups, alcohols are interesting polar solvents, self-associated through hydrogen bonding creating multimers of different degrees. And the dipolar association of alcohols decreases when they are mixed with aromatic hydrocarbons, due to some sort of specific intermolecular interactions between alcohols and aromatic hydrocarbons [8]. 1-Hexanol is a linear primary alcohol. It is formed as an intermediate during the catalytic transformation of cellulose. 1-Hexanol is produce from coconut oil and palm oils. It is used in the production of antiseptics, fragrances and perfumes. 1-Hexanol is also used as a solvent in the production of plasticizers. 1- Hexanol has been used as an odorant to study olfactory responses and to thin the dielectric layer of poly (PVP).

1-Hexanol is believed to be a component of the odour of freshly mown grass. It is used in the perfume industry and as a flavouring agent. 1-Hexanol is found in many plants, some of which are lemon, tea, yellow bell pepper, and hyssop. 1-Hexanol is a common constituent of essential oils (e.g. orange-peel oil) [9]. Benzene is a chemical that is a colorless, light yellow liquid at room temperature. It has a sweet odor and is highly flammable liquid with a sweet smell and is partially responsible for the aroma of gasoline. Benzene evaporates into the air very quickly. Its vapor is heavier than air and may sink into low-lying areas. Benzene dissolves only slightly in water and will float on top of water. Benzene are used to make some types rubbers lubricants, dyes, detergents, drug, explosive, pesticides, spot removers and other products [10]. Literature survey further revealed that although many attempts have already been made to study the binary mixtures of alcohols and aromatic hydrocarbons, systematic studies focusing their dependence on composition and number position as well as length of substituent on aromatic hydrocarbons are still scarce. In this paper I have reported on densities, excess molar volumes, interaction

parameter of the binary mixture of 1-Hexanol + Benzene.

MATERIALS AND METHODS

1-Hexanol: Aldrich, mole fraction purity > 0.99%, Benzene: Merck, mole fraction purity > 0.996, were kept over molecular sieves for 3-5 weeks and binary mixture of various compositions were prepared by mass mixing pure components at different proportions with the help of an electronic balance (B 204-S, METTLER TOLEDO) accurate up to ±0.0003 g. Densities, ρ were measured by using a 10 cm^3 bi-capillary pycnometer being calibrated previously with twice distilled water. The flow time of liquids was recorded by an electronic stopwatch reading up to ±0.02 s. For all measurements a thermostatic water bath (Thermo Haake) controlled up to± 0.03 K was used. The mole fraction was estimated accurate up to 10^{-4}, while the uncertainty in measured ρ were $\pm 1.29\times10^{-4}$ $g.cm^{-3}$. The purities were further checked by comparing measured ρ of pure liquids with the literature data as tabulated in Table 1.

Table 1: Comparison of experimental densities (ρ /$g.cm^{-3}$) pure liquids with literature values at 303.15 K.

S. No	Liquids	Experimental values	Literature values
1.	1-Hexanol	0.8113	0.8100
2.	Benzene	0.8674	0. 8680

RESULTS AND DISCUSSION

Excess molar volumes

Excess molar volumes, V_m^E for a solution is expressed as [11]

$$V_m^E = V_m - (x_1 V_1^* + x_2 V_2^*) \quad \text{(1)}$$

where, V_m is the molar volume of the mixture and V^* are the molar volumes x_1 and x_2 are the mole fractions of the pure component 1 and 2 respectively. V_m^E of the binary mixtures were calculated from experimental densities of pure liquids and their mixtures by using the equation [12]:

$$V_m^E = \left[\frac{x_1 M_1 + x_2 M_2}{\rho}\right] - \left[\frac{x_1 M_1}{\rho_1} + \frac{x_2 M_2}{\rho_2}\right] \quad \text{(2)}$$

Here, ρ is the density of the mixture, M_1 and M_2 represent the molar masses and ρ_1 and are ρ_2 the densities of components 1 and 2, respectively. V_m^E values for the system of 1- Hexanol and Benzene are listed in Table 2. against mole fraction of aromatic hydrocarbons, x_2 at 303.15 K. The results were fitted by the Redlich-Kister equation [13]:

$$Y^E = [(1-x_1)\ x_2 \sum_{i=0}^{n} Ai\ (1 - 2 \cdot x_1)^i \quad \text{(3)}$$

The standard deviation, σ followed the equation:

$$\sigma = \left[\frac{\Sigma(Yexp - Ycal)^2}{n-p-2}\right]^{1/2} \quad \text{(4)}$$

Where, $Y^E \equiv V_m^E$ and *Ai* is the i-th polynomial fitting coefficient, *Yexp* and *Ycal* are the experimental and calculated of properties, n the total number of compositions for a particular system and *p* is the number of coefficients. In the hole range of composition are to be found positive values.

Table 2: Densities, ρ ($g.cm^{-3}$) and Excess molar volumes, V_m^E ($cm^3.mol^{-1}$) of the systems of 1-Hexanol (x_1)+ Benzene (x_2), for different molar ratios at 303.15 K.

Mole fraction (x2)	Densities (ρ)	Excess molar volumes (V_m^E)
0.0000	0.8113	0.0000
0.1041	0.8198	0.0657
0.2110	0.8254	0.0745
0.3201	0.8297	0.0954
0.4005	0.8354	0.1142
0.5034	0.8397	0.1345
0.6158	0.8452	0.1237
0.7047	0.8495	0.1058
0.8112	0.8564	0.0988
0.9005	0.8602	0.7897
1.0000	0.8674	0.0000

The above results have been explained as follows. When small amount of 1-Hexanol is added to aromatic hydrocarbons Benzene separately, it is expected that it would disperse within aromatic hydrocarbons causing depolymerization of the network structures and disrupt their H-bonding and resulting into volume expansion. So that, V_m^E become positive for the system [14-15]. The dispersive forces [16] has established that with the increased steric hindrance in the aromatic hydrocarbons the positive becomes more positive.

Partial molar volumes

The partial molar volume of the i-th component for a solution, *Vi* , is defined as [17-22]:

$$V_i = \left(\frac{\partial V_m^E}{\partial n_i}\right)_{T,\, nJ} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

Considering equation (1) in (5) equations obtained for the partial molar volumes V_1 and V_2 of components 1 and 2 respectively are:

$$V_1 = V_1^* + V_m^E - x_2\left(\frac{\partial V_m^E}{\partial x_2}\right) \ldots\ldots\ldots\ldots(6)$$

$$V_2 = V_2^* + V_m^E - (1- x_2)\left(\frac{\partial V_m^E}{\partial x_2}\right)_T \ldots\ldots\ldots(7)$$

Following the procedure [23] , V_1 and V_2 were obtained as:

$$V_1 = V_1^* + x_2^2 \sum_{i=0}^{n} A_i (1-2x_2)^i + 2x_2^2 (1-x_2) \sum_{i=0}^{n} iA_i (1-2x_2)^{i-1} \ldots\ldots\ldots(8)$$

$$V_2 = V_2^* + (1-x_2)^2 \sum_{i=0}^{n} A_i (1-2x_2)^i + 2x_2^2 (1-x_2)^2 \sum_{i=0}^{n} iA_i (1-2x_2)^{i-1} \ldots\ldots(9)$$

The results are as listed in Table 3. The difference between partial molar volume, *Vi* and molar volume V_i^* of each of component was also estimated at 303.15 K and thus the values obtained for (Vi - V_i^*) are both the components, these differences are positive for the system, indicating that there is volume expansion in the system. This is exactly in support of observed values of V_m^E experimentally.

Table 3: Partial molar volumes of component 1, V_1 ($cm^3.mol^{-1}$) and of component 2, V_2 ($cm^3.mol^{-1}$) in the systems of 1-Hexanol and Benzene for different molar ratios at 303.15 K

Mole fraction (x_2)	Partial molar volumes(V_1)	Partial molar volumes(V_2)
0.0000	117.584	115.214
0.1041	117.654	115.415
0.2110	117.745	115.568
0.3201	117.812	115.748
0.4005	117.947	115.845
0.5034	118.254	115.987
0.6158	118.412	116.147
0.7047	118.587	116.354
0.8112	118.678	116.544
0.9005	118.787	116.678
1.0000	118.954	116.845

The adjustable parameters and standard deviations are as given in Table .4

Table 4: Fitting coefficients of polynomial equation (3) and standard deviations, σ in equation (4) for the system of 1-Hexanol (x_1) + Benzene (x_2) for different molar ratios at 303.15 K

Property	A_0	A_1	A_2	A_3	A_4	σ
V / cm^3 mol^{-1}	0.5427	-0.7485	-0.3548	-0.0875	0.8475	0.0074

The values of V_m^E indicated that all the species get favorable conditions to flow. This is because addition of 1-Hexanol to Benzene causes mainly dispersion due to break up of weak forces. Also, aromatic hydrocarbons with longer chain lengths encounter less inconvenience to flow even through intermolecular H-bonded species may also present in the solution.

CONCLUSION

Density for the binary mixture of 1-Hexanol + Benzene system at 303.15 K have measured and calculated V_i, V_i^* and V_m^E. The values of V_m^E were found to be positive in the whole range of composition. These positive values are observed in the alcohol-rich region which may be suggested as due to depolymerization of the network structures and disrupt their H-bonding and resulting into volume expansion.

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