Thermodynamic Properties of the Binary Mixture of Hexan-1-ol with *m*-Xylene at $T = (303.15, 313.15, \text{and } 323.15)$ K

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Volumetric and viscometric properties of the binary mixture of hexan-1-ol with *m*-xylene at $T = (303.15, 313.15, \text{and } 323.15)$ K have been investigated. The excess volumes and viscosity deviations from the mole fraction average were calculated and correlated by a Redlich−Kister type equation.

Introduction

The nature and type of interactions in binary (or multicomponent) solvent systems are essential to understanding their behavior in different analytical applications for fetched, process engineering design applications and other related areas.[1−4] This work is a continuation of our research on the physical properties of binary organic liquid mixtures,[5−8] and here we report the density and viscosity of the binary system composed of hexan-1-ol and *m*-xylene at $T = (303.15, 313.15, \text{and } 323.15)$ K. Interaction between hexan-1-ol and *m*-xylene is compared with that reported for hexan-1-ol with *o*-xylene.[8]

Experimental Section

Hexan-1-ol and *m*-xylene from Merck-Schuchard, Germany (0.98 mass fraction purity), were used without further purification. Caution was taken to prevent evaporation of the solutions after preparation.

All binary mixtures were prepared by mass on an analytical balance with an uncertainty of ± 0.0001 g and operating in a drybox. Mixtures were made just before use. A 10 mL bicapillary pycnometer and an A-type Ostwald viscometer, previously calibrated with redistilled water, were used. The temperature was controlled by a thermostatic water bath, and the uncertainty in measurements was ± 0.05 K. For all mixtures and pure solvents, triplicate measurements were performed, and the average of these values was taken. The average uncertainties were ± 0.0002 g·cm^{-3} for density and ± 0.005 mPa·s for viscosity.

The solvent purity was ascertained by comparing the densities and viscosities of the liquids with the available literature data (Table 1). There is fairly good agreement between our data and the previously reported values.

Table 1. Comparison of Experimental Densities, ρ, and Viscosities, η, of Pure Liquids with Literature Values at $T = (303.15 \text{ and } 313.15)$ K

		ρ/g·cm^{-3}			η/mPa·s		
liquid (s)	T/K	exptl	lit.	ref	exptl	lit.	ref
hexan-1-ol	303.15	0.8119	0.8120	16	3.829	3.763	17
			0.8121	18		3.769	18
			0.8115	19		3.84	16
						3.861	19
	313.15	0.8046	0.8046	16	2.879	2.90	16
			0.8046	18		2.89	20
			0.80428	21		2.934	22
						2.966	21
	323.15	0.7975	0.7972	16	2.215	2.23	16
			0.7979	18		2.21	20
m-xylene	303.15	0.8555	0.8553	23	0.550	0.547	24
			0.85561	24		0.555	23
			0.85587	25		0.556	25
	313.15	0.8470	0.8471	26	0.494	0.508	26
			0.84717	27			
	323.15	0.8384	0.8389	28	0.447	0.447	28

Results and Discussion

Hexan-1-ol is an aliphatic polar solvent with strong self-associating nature via hydrogen bonding and van der Waals interactions.[9,10] On the contrary, *m*-xylene is a nonassociating solvent, but a favorable interaction with the hydroxyl group of hexan-1-ol is possible due to the presence of aromatic rings with delocalized π-electrons.[11] The experimental density, excess molar volumes, viscosity, and viscosity deviation for the binary mixtures of hexan-1-ol with *m*-xylene at (303.15, 313.15, and 323.15) K are listed in Table 2 against the mole fraction, x_1, of hexan-1-ol.

The excess molar volumes, V_m^E, for the binary mixtures were calculated from the density data with the following formula

$$V_m^E = [(x_1M_1 + x_2M_2)/\rho - \{(x_1M_1)/\rho_1 + (x_2M_2)/\rho_2\}] \quad (1)$$

where x_1, M_1, and ρ_1 represent, respectively, mole fraction, molar mass, and density of hexan-1-ol, and x_2, M_2, and ρ_2 are the corresponding quantities of *m*-xylene. ρ is the density of the binary mixtures. Figure 1 illustrates the excess molar volumes for the binary mixtures varying with the mole fraction of hexan-1-ol (x_1) at $T = (303.15, 313.15, \text{and } 323.15)$ K. As it shows, for the whole range of compositions, the values of V_m^E are positive for the binary systems of hexan-1-ol with *m*-xylene. The expansion of volume may be due to the disintegration of associated molecules of hexan-1-ol through disruption of H-bonding in the solution system containing the nonpolar component *m*-xylene.

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Table 2. Composition, Experimental Densities, ρ, Excess Molar Volumes, V_m^E, Viscosities, η, and Viscosity Deviation, $\Delta\eta$, for the Binary Mixtures of Hexan-1-ol with *m*-Xylene at T = (303.15, 313.15, and 323.15) K

Densities and Excess Molar Volumes of Hexan-1-ol (1) + *m*-Xylene (2)						
	T/K = 303.15		T/K = 313.15		T/K = 323.15	
	ρ	V_m^E	ρ	V_m^E	ρ	V_m^E
x_1	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}
0.0000	0.8555	0.0000	0.8470	0.0000	0.8384	0.0000
0.1002	0.8506	0.0695	0.8420	0.1046	0.8332	0.1611
0.2002	0.8459	0.1137	0.8373	0.1685	0.8287	0.2198
0.3007	0.8413	0.1423	0.8329	0.1864	0.8245	0.2313
0.4001	0.8370	0.1355	0.8287	0.1829	0.8205	0.2203
0.5000	0.8327	0.1272	0.8246	0.1624	0.8165	0.2075
0.5999	0.8285	0.1054	0.8205	0.1434	0.8126	0.1804
0.6999	0.8244	0.0694	0.8165	0.1097	0.8087	0.1537
0.7999	0.8203	0.0347	0.8125	0.0773	0.8049	0.1124
0.8999	0.8161	0.0169	0.8086	0.0305	0.8011	0.0721
1.0000	0.8119	0.0000	0.8046	0.0000	0.7975	0.0000

Viscosities and Deviations of the Viscosity of Hexan-1-ol (1) + *m*-Xylene (2)						
	η	$\Delta\eta$	η	$\Delta\eta$	η	$\Delta\eta$
x_1	mPa·s	mPa·s	mPa·s	mPa·s	mPa·s	mPa·s
0.0000	0.550	0.000	0.494	0.000	0.447	0.000
0.1002	0.598	−0.070	0.531	−0.059	0.474	−0.051
0.2002	0.683	−0.129	0.598	−0.106	0.528	−0.088
0.3007	0.800	−0.186	0.689	−0.150	0.601	−0.123
0.4001	0.954	−0.242	0.807	−0.194	0.693	−0.156
0.5000	1.161	−0.291	0.965	−0.229	0.814	−0.181
0.5999	1.442	−0.319	1.173	−0.250	0.970	−0.198
0.6999	1.833	−0.306	1.457	−0.240	1.179	−0.192
0.7999	2.357	−0.240	1.833	−0.191	1.448	−0.160
0.8999	3.032	−0.121	2.309	−0.105	1.797	−0.091
1.0000	3.829	0.000	2.879	0.000	2.215	0.000

The viscosity deviations, $\Delta\eta$, have been calculated from the following relationship

$$\Delta\eta = \eta - \exp(x_1 \ln \eta_1 + x_2 \ln \eta_2) \quad (2)$$

where η_1 and η_2 are the viscosities of the pure components at the experimental temperatures, and x_1 and x_2 are their respective mole fractions in the mixture. η is the viscosity of the binary mixtures. The trend of $\Delta\eta$ for the binary mixtures of hexan-1-ol with *m*-xylene as a function of the binary composition at T = (303.15, 313.15, and 323.15) K is shown in Figure 2. The viscosity of a mixture according to Kauzman and Eyring[12] strongly depends on the entropy of the mixture, which is related to the liquids structure and bond enthalpy, and consequently with molecular interactions between the components of the mixture. In the binary system of hexan-1-ol with *m*-xylene, there must be geometrical effects of molecules which results in negative deviations of viscosity. The negative values observed for $\Delta\eta$ of the binary mixtures correspond to a system containing an associated component.[13]

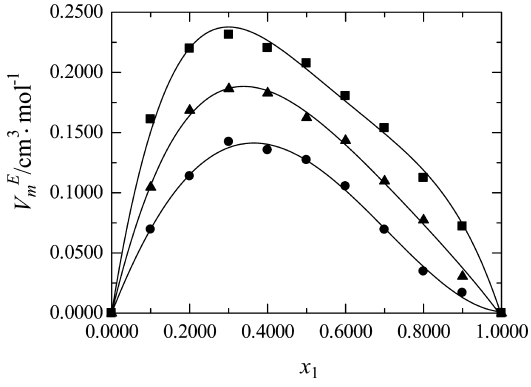

Figure 1. Excess molar volumes for hexan-1-ol (1) + *m*-xylene (2): ●, 303.15 K; ▲, 313.15 K; ■, 323.15 K.

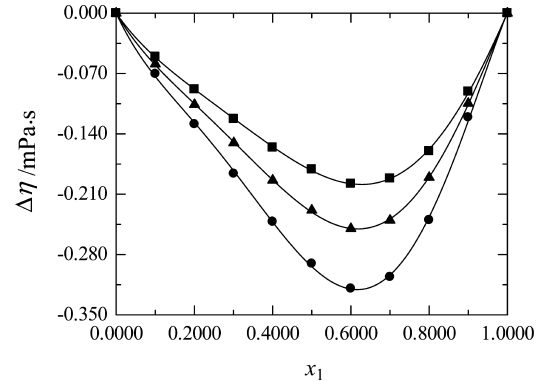

Figure 2. Viscosity deviations for hexan-1-ol (1) + *m*-xylene (2): ●, 303.15 K; ▲, 313.15 K; ■, 323.15 K.

Table 3. Coefficients, A_i, of the Redlich−Kister Equation (Equation 3), Expressing V_m^E and $\Delta\eta$, and Standard Deviation, σ, for the Binary Mixtures of Hexan-1-ol with *m*-Xylene at T = (303.15, 313.15, and 323.15) K

T/K	A_0	A_1	A_2	A_3	σ
Correlated Results for Excess Volumes of Hexan-1-ol (1) + *m*-Xylene (2)					
303.15	0.5073	−0.4117	0.0749	−0.0406	0.00425
313.15	0.6682	−0.4254	0.2068	−0.1401	0.00450
323.15	0.8113	−0.4175	0.6859	−0.3379	0.00425
Correlated Results for Viscosity Deviations of Hexan-1-ol (1) + *m*-Xylene (2)					
303.15	−1.1763	−0.8422	0.1138	0.7573	0.00383
313.15	−0.9235	−0.6057	0.0025	0.4529	0.00161
323.15	−0.7307	−0.4594	−0.1051	0.2680	0.00149

The excess molar volumes (V_m^E) or viscosity deviation ($\Delta\eta$) were correlated by a Redlich−Kister[14] type equation

$$\delta = x_1 x_2 \sum_{i=0}^{n} A_i (1 - 2x_1)^i \quad (3)$$

where δ refers to V_m^E or $\Delta\eta$ and x_1 and x_2 are the mole fractions of hexan-1-ol and *m*-xylene, respectively. The coefficients of A_i are obtained by fitting the equation to the experimental values with a least-squares algorithm (Table 3).

The binary solvent system of hexan-1-ol with *m*-xylene has higher excess volume and lower excess viscosity than that reported for hexan-1-ol with *o*-xylene.[8] It indicates that stronger interaction of hexan-1-ol with *m*-xylene than *o*-xylene resulted, may be due to the steric effect.

Excess molar volumes for the hexan-1-ol and *m*-xylene binary system at 298.15 K were reported by Rodriguez-Nuñez et al.[15] However, no literature data are available with which to compare the present results for hexan-1-ol with *m*-xylene at T = (303.15, 313.15, and 323.15) K.

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