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Viscosities, densities, speeds of sound and refractive indices of binary mixtures of o-xylene, m-xylene, p-xylene, ethylbenzene and mesitylene with 1-decanol at 298.15 and 308.15 K

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ABSTRACT

The viscosities η, densities ρ, speeds of sound u and refractive indices n_D of binary mixtures of 1-decanol with o-xylene, m-xylene, p-xylene, ethylbenzene and mesitylene have been measured over the entire range of composition at 298.15 and 308.15 K and at atmospheric pressure. Excess molar volumes V^E, deviations of isentropic compressibilities $\Delta\kappa$, deviations of the speeds of sound Δu, viscosity deviations $\Delta\eta$, excess free energies of activation for viscous flow ΔG^{*E} and deviations of refractive indices Δn_D have been calculated from the density ρ, speed of sound u, viscosity η and refractive index n_D data. The calculated excess and deviation functions have been fitted to the Redlich–Kister polynomial equations and the results analyzed in terms of molecular interactions and structural effects. The viscosity data have been correlated using McAllister's three body interaction model at different temperatures.

1. Introduction

The extraction of benzene, toluene, ethylbenzene and xylene from refinery products such as naphtha, kerosene and fuel jets is very important in the petrochemical industry. For this purpose, the information about the thermodynamic, transport, acoustic and optical properties of pure liquids and liquid mixtures containing aromatic hydrocarbons and their dependence on composition and temperature is quite essential. It is, therefore, interesting to carry out the systematic investigations of these properties for the binary liquid mixtures of 1-alkanols with organic compounds [1–5].

Alkanols are polar and self-associated liquids and the dipolar association of alkanols decreases when they are mixed with aromatic hydrocarbons, due to some sort of specific intermolecular interactions between alkanols and aromatic hydrocarbons. In an attempt to explore the nature of interactions occurring between 1-alkanols and aromatic hydrocarbons, the viscosities η, densities ρ, speeds of sound u and refractive indices n_D of binary liquid mixtures of 1-decanol with o-xylene, m-xylene, p-xylene, ethylbenzene and mesitylene have been measured over the entire range of composition at 298.15 and 308.15 K and at atmospheric pressure. Excess molar volumes V^E, deviation of isentropic compressibilities $\Delta\kappa$, deviation of the speeds of sound u^D, viscosity deviations $\Delta\eta$, excess free energies of activation for viscous flow ΔG^{*E} and deviations of refractive index Δn_D have been calculated from the density ρ, speed of sound u, viscosity η and refractive index n_D data. The calculated excess and deviation functions have been fitted to the Redlich–Kister polynomial equation and the results analyzed in terms of molecular interactions and structural effects. The viscosity data have been correlated using McAllister's three body interaction model at different temperatures.

2. Experimental

2.1. Materials

The mass fraction purity of the liquids from S.D. fine Chemical Ltd. was as follows: 1-decanol>99.0%, o-xylene>99.5%, m-xylene>99.0%, p-xylene>99.0%, ethylbenzene>99.7% and mesitylene>99.7%. Prior to experimental measurements, all the liquids were used after double-distillation, and partially degassed with a vacuum pump under nitrogen atmosphere. The purity of these solvents was ascertained by comparing the measured densities ρ, speeds of sound u, viscosities η and refractive indices n_D of the components at 298.15 and 308.15 K with the available literature [6–16] presented in Table 1.

2.2. Apparatus and procedures

All the liquid mixtures were prepared by weighing appropriate amounts of pure liquids on an Afcoset-ER-120A electronic balance, with a precision of ±0.05 mg by syringing each component into airtight stoppered bottles to minimize evaporation losses. The accuracy of the mole fraction was ±0.0001.

Densities ρ and speeds of sounds u of the pure liquids and their mixtures were measured with density and sound speed analyzer

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Table 1
Comparison of density ρ, speed of sound u, viscosity η and refractive index n_D of pure liquids with the corresponding literature values at 298.15 and 308.15 K.

Pure liquid	T/K	ρ/kg m^{-3}		u/m s^{-1}		η/mPa s		n_D	
		Exp	Lit	Exp	Lit	Exp	Lit	Exp	Lit
1-Decanol	298.15	826.53	826.57[a]	1379	1379.7[b]	11.819	11.825[g]	1.4345	1.4345[j]
	308.15	819.67	819.62[b]	1345	1345.8[b]	8.132	8.135[g]	1.4305	1.4303[j]
o-Xylene	298.15	875.28	875.53[c]	1348	1349.4[c]	0.755	0.756[c]	1.5028	1.5029[k]
	308.15	866.82	867.05[d]	1308		0.674	0.676[h]	1.4975	1.4975[k]
m-Xylene	298.15	859.87	859.77[c]	1320	1321.0[c]	0.583	0.581[c]	1.4947	1.4948[k]
	308.15	851.24	851.45[d]	1279		0.531	0.533[h]	1.4888	1.4896[k]
p-Xylene	298.15	856.61	856.62[c]	1310	1310.0[c]	0.609	0.611[c]	1.4933	1.4933[k]
	308.15	847.88	848.12[d]	1269	1268.0[f]	0.548	0.547[i]	1.4877	1.4881[k]
Ethylbenzene	298.15	862.43	862.64[e]	1319		0.635		1.4928	1.4932[e]
	308.15	853.61		1278		0.558		1.4868	
Mesitylene	298.15	860.86	861.06[c]	1336	1336.9[c]	0.660	0.661[c]	1.4968	1.4969[k]
	308.15	852.66	853.63[d]	1296		0.583		1.4908	1.4918[k]

[a] [6] O. Kiyohara, G.C. Benson.
[b] [7] M. Dzida, P. Goralski.
[c] [8] J.A. Al-Kandary, A.S. Al-Jimaz, A.H.M. Abdul-Latif.
[d] [9] A.K. Nain, R. Sharma, A. Ali, S. Gopal.
[e] [10] J.A. Riddick, W.B. Bunger, T.K. Sakano.
[f] [11] O. Kiyohara, K. Arakawa.
[g] [12] A.S. Al-Jimaz, J.A. Al-Kandary, A.H.M. Abdul-Latif.
[h] [13] A. Ali, A.K. Nain, D. Chand, R. Ahmad.
[i] [14] T.M. Aminabhavvi, L.S. Manjeshwar, S.B. Halligudi, R.H. Balundgi.
[j] [15] J. Ortega.
[k] [16] A.K. Nain.

apparatus (Anton Paar DSA 5000) operated in the static mode and automatically thermostated within ±0.001 K using the Peltier element. Before each series of measurements, the calibration of the apparatus was carried out at working temperature by measuring densities and speeds of sound of double-distilled water, benzene and toluene respectively. The experimental values conform closely to their corresponding literature [6–16] values, to an uncertainty of ±0.02 kg m^{-3} and ±1 m s^{-1} for the density and speed of sound, respectively.

Kinematic viscosities ν at 298.15 and 308.15 K were measured with a modified Ubbelohde suspended-level viscometer. The viscometer was suspended in a thermostated water bath maintained to ±0.01 K. An electronic digital stop watch with an uncertainty of ±0.01 s was used for flow time measurements. At least four flow time measurements were performed for each composition and temperature, and the results were averaged. Calibration of the viscometer was carried out with high purity benzene, toluene and cyclohexane. The equation for viscosity, according to Poiseuille's law is

$$\eta = \rho\nu = \rho(kt - c/t) \tag{1}$$

where k and c are the viscometer constants and t, η and ν are the efflux time, dynamic viscosity and kinematic viscosity respectively. The uncertainty in the viscosity measurements was of the order of ±0.003 mPa s.

Refractive indices $n_{D,}$ were measured with a thermostatic Abbe Refractometer (Erma, A-302A) using sodium-D-line with an error less than ±0.0001 units at 298.15 and 308.15 K. The temperature in the refractometer was regulated by using a circulation pump connected with a constant temperature water bath with ±0.01 °C stability. Calibration of the instrument was carried out at the working temperature by measuring the refractive indices of double-distilled water, benzene and toluene. The uncertainty in the refractive index measurements was of the order of ±0.0002.

3. Results and discussion

The experimental results of densities ρ, speeds of sound u, viscosities η and refractive indices n_D for binary liquid mixtures at 298.15 and 308.15 K are listed in Table 2.

The excess molar volumes V^E of the binary mixtures were calculated from the densities of the pure liquids and their mixtures using the equation

$$V^E = \sum_{i=1}^{2} x_i M_i \left(\rho^{-1} - \rho_i^{-1}\right) \tag{2}$$

where ρ is the density of the mixtures and x_i, M_i, and ρ_i are the mole fraction, molecular weight and the density of pure components, respectively.

From the results of densities and speeds of sound, the isentropic compressibilities κ_S were calculated using the Newton–Laplace equation

$$\kappa_S = 1/u^2\rho \tag{3}$$

The corresponding deviation of isentropic compressibilities $\Delta\kappa$ were obtained from the relation

$$\Delta\kappa = \kappa_S - \kappa_S^{id} \tag{4}$$

where κ_S is the experimental compressibility and κ_S^{id} is the ideal value of isentropic compressibility and was calculated from the Benson and Kiyohara relation [6]

$$\kappa_S^{id} = \sum_{i=1}^{2} \phi_i \left[\kappa_{S,i} + \frac{TV_i\left(\alpha_i^2\right)}{C_{P,i}}\right] - \left\{\frac{T\left(\sum_{i=1}^{2} x_i V_i\right)\left(\sum_{i=1}^{2} \phi_i \alpha_i\right)^2}{\sum_{i=1}^{2} x_i C_{P,i}}\right\} \tag{5}$$

Here, C_{Pi} and α_i are the molar heat capacity and the thermal expansion coefficient of the pure components, respectively. The values of C_{Pi} were obtained from literature [8,12,17] and these values are presented in Table 3. The thermal expansion coefficient α has been calculated from the equation $\alpha = -\rho^{-1}(\partial\rho/\partial T)_P$. The α values are given in Table 3.