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Viscosities, Densities, and Ultrasonic Velocities of 3-Pentanone + Ethylbenzene and 3-Pentanone + *o*-Xylene at (293.15, 303.15, and 313.15) K

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The densities, viscosities, and ultrasonic velocities of 3-pentanone with ethylbenzene and *o*-xylene have been determined at (293.15, 303.15, and 313.15) K over the whole composition range. Excess volume (V^E), excess compressibility (K_S^E), and deviations in viscosity ($\Delta\eta$) were calculated.

Introduction

The studies of viscosity, density, and ultrasonic velocity of binary mixtures along with other thermodynamic properties are being increasingly used as tools for the investigation of the properties of pure components and the nature of intermolecular interactions between the liquid mixture constituents.

In recent years, there has been a considerable advancement in the experimental investigation of the excess thermodynamic properties of liquid mixtures. A survey of the literature[1] shows that few attempts have been made to study binary mixtures of 3-pentanone. In the present study, the measurements of densities, viscosities, and ultrasonic velocities for 3-pentanone with ethylbenzene and *o*-xylene have been made at (293.15, 303.15, and 313.15) K.

Experimental Section

3-Pentanone (Merck Schuchardt), ethylbenzene (Fluka), and *o*-xylene (E. Merck, India) were purified using standard procedures[2] and stored over molecular sieves. The purity was checked by comparing the measured densities and viscosities with those reported in the literature, as shown in Table 1.

Densities were measured using a calibrated bicapillary pycnometer having an accuracy of $\pm 1 \times 10^{-4}$ g·cm^{-3}. The mole fraction of each mixture was obtained to an accuracy of $\pm 1 \times 10^{-4}$.

Viscosities were determined using a modified Ubbelohde viscometer, as described earlier.[3] From the measured values of ρ and efflux time t, the viscosity was calculated using the relation

$$\eta/\rho = At + B/t \tag{1}$$

where A and B are viscometer constants.

The values of the constants were obtained by measuring the flow time with triply distilled water and twice distilled benzene. The flow measurements were made with an electronic stopwatch with a precision of ±0.01 s. An average of three or four sets of flow times for each liquid or liquid mixture was taken for the purpose of calculation of viscosity. The uncertainty in the values is within ±0.003 mPa·s.

Table 1. Physical Properties of the Pure Components at Different Temperatures

		ρ/g·cm^{-3}		η/mPa·s	
component	T/K	expt	lit.	expt	lit.
ethylbenzene	293.15	0.8674	0.866 96[6]	0.6793	0.678 3[2]
	303.15	0.8565	0.858 28[6]	0.6006	0.601 87[2]
	313.15	0.8489	0.849 44[6]	0.5355	0.535 82[2]
o-xylene	293.15	0.8802	0.880 20[6]	0.8092	0.809 00[2]
	303.15	0.8718	0.871 86[6]	0.7172	0.717 16[2]
	313.15	0.8632	0.863 17[6]	0.6292	0.629 28[2]
3-pentanone	293.15	0.8144	0.814 40[6]	0.4714	0.471 32[2]
	303.15	0.8047	0.804 66[2]	0.4231	0.423 00[2]
	313.15	0.7949	0.794 94[2]	0.3799	0.379 97[2]

Ultrasonic velocities were determined using an Ultrasonic time intervalometer (UTI-101) with reproducibility within ±0.1 ms^{-1}.

All the measurements were made at a constant temperature with the help of a circulating type cryostat where the temperature was controlled to ±0.02 K.

Experimental Results and Correlations

The experimental values of viscosity, η, density, ρ, and ultrasonic velocity, u, are reported in Tables 2 and 3.

Deviations in viscosity, $\Delta\eta$, were obtained by using the following relation

$$\Delta\eta = \eta_m - (x_1\eta_1 + x_2\eta_2) \tag{2}$$

where η_m is the viscosity of the mixture and η_1 and η_2 are the viscosities of pure components 1 and 2, respectively.

The molar volume V_m was calculated using the relation

$$V_m = (x_1M_1 + x_2M_2)/\rho_m \tag{3}$$

where x_1, x_2, M_1, and M_2 are the mole fractions and molecular weights of components 1 and 2, respectively, and ρ_m is the mixture density. The excess volumes (V^E) for these binary mixtures were obtained using the relation

$$V^E = x_1M_1(1/\rho_m - 1/\rho_1) + x_2M_2(1/\rho_m - 1/\rho_2) \tag{4}$$

where ρ_1 and ρ_2 are the densities of pure components 1 and 2.

The value of the mixture density, ρ_m, and the ultrasonic velocities, u, were used to calculate the isentropic com-

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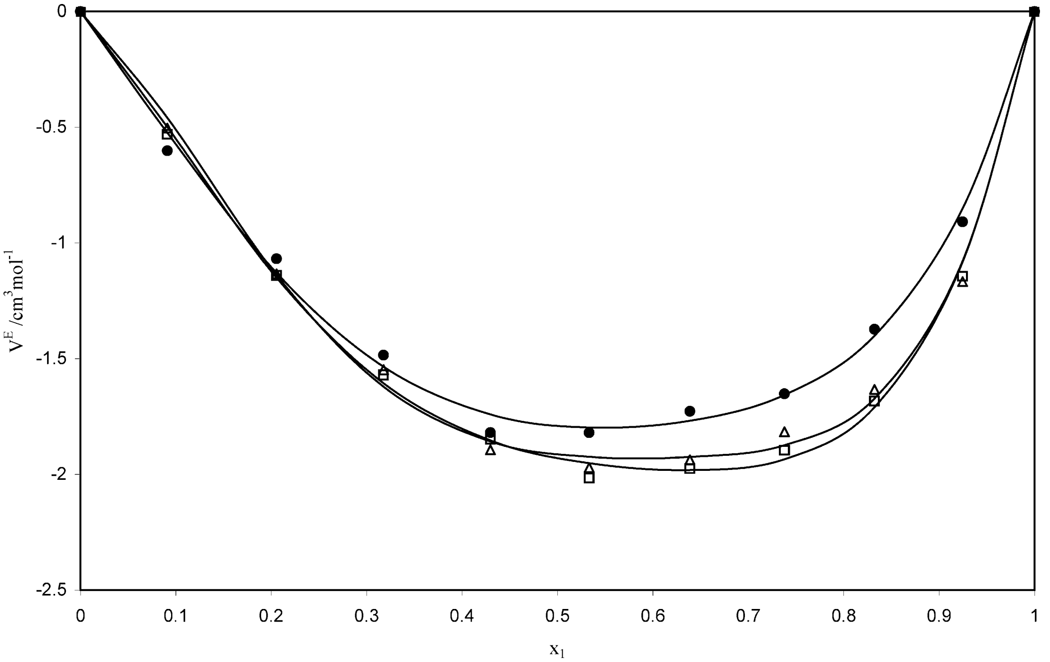

Figure 1. Excess molar volume, V^E ($cm^3{\cdot}mol^{-1}$), for the system 3-pentanone (1) + ethylbenzene (2) at (●) 20 °C, (△) 30 °C, and (□) 40 °C.

Table 2. Density, *ρ*, Ultrasonic Velocity, *u*, Viscosity, *η*, and Compressibility, K_S, for the 3-Pentanone (1) + Ethylbenzene (2) System at Different Temperatures

x_1	ρ / $g{\cdot}cm^{-3}$	u / $m{\cdot}s^{-1}$	η / mPa·s	$10^{12}K_S$ / Pa^{-1}
		$T = 293.15$ K		
1.0000	0.8144	1230.7	0.4714	810.7
0.9245	0.8260	1240.3	0.4811	786.9
0.8322	0.8350	1251.0	0.4975	765.2
0.7378	0.8425	1263.0	0.5160	744.0
0.6387	0.8485	1275.0	0.5340	724.9
0.5331	0.8548	1287.0	0.5574	706.2
0.4296	0.8601	1298.0	0.5789	690.0
0.3176	0.8632	1309.6	0.6015	675.4
0.2055	0.8655	1319.0	0.6250	664.1
0.0911	0.8670	1328.5	0.6538	653.1
0.0000	0.8674	1333.4	0.6793	648.4
		$T = 303.15$ K		
1.0000	0.8047	1197.8	0.4231	866.1
0.9245	0.8180	1206.6	0.4309	839.6
0.8322	0.8268	1217.5	0.4410	815.9
0.7378	0.8334	1230.0	0.4540	793.1
0.6387	0.8396	1242.0	0.4690	772.1
0.5331	0.8453	1252.3	0.4860	754.3
0.4296	0.8499	1264.5	0.5046	735.8
0.3176	0.8528	1272.2	0.5281	724.5
0.2055	0.8551	1281.9	0.5539	711.6
0.0911	0.8559	1290.2	0.5795	701.8
0.0000	0.8565	1295.7	0.6006	695.4
		$T = 313.15$ K		
1.0000	0.7949	1159.1	0.3799	936.4
0.9245	0.8080	1172.5	0.3800	900.2
0.8322	0.8175	1184.4	0.3880	872.0
0.7378	0.8245	1195.0	0.3990	849.3
0.6387	0.8306	1206.0	0.4110	827.8
0.5331	0.8366	1217.5	0.4247	806.4
0.4296	0.8408	1227.2	0.4429	789.7
0.3176	0.8445	1237.2	0.4642	773.6
0.2055	0.8470	1246.6	0.4881	759.7
0.0911	0.8483	1254.5	0.5116	749.0
0.0000	0.8489	1259.8	0.5355	742.2

Table 3. Density, *ρ*, Ultrasonic Velocity, *u*, Viscosity, *η*, and Compressibility, K_S, for the 3-Pentanone (1) + *o*-Xylene (2) System at Different Temperatures

x_1	ρ / $g{\cdot}cm^{-3}$	u / $m{\cdot}s^{-1}$	η / mPa·s	$10^{12}K_S$ / Pa^{-1}
		$T = 293.15$ K		
1.0000	0.8144	1230.7	0.4714	810.7
0.9242	0.8263	1250.9	0.4882	773.4
0.8283	0.8368	1266.2	0.5100	745.4
0.7329	0.8450	1279.4	0.5370	723.0
0.6363	0.8521	1292.2	0.5680	702.8
0.5338	0.8595	1306.0	0.6001	682.2
0.4298	0.8653	1318.8	0.6360	664.5
0.3191	0.8711	1333.5	0.6750	645.6
0.2073	0.8750	1345.1	0.7182	631.6
0.0955	0.8780	1357.0	0.7649	618.5
0.0000	0.8802	1365.6	0.8092	609.2
		$T = 303.15$ K		
1.0000	0.8047	1197.8	0.4231	866.0
0.9242	0.8170	1213.0	0.4333	831.9
0.8283	0.8291	1229.0	0.4481	798.5
0.7329	0.8373	1245.0	0.4719	770.5
0.6363	0.8440	1255.8	0.4970	751.3
0.5338	0.8505	1272.0	0.5271	726.6
0.4298	0.8573	1287.0	0.5620	704.2
0.3191	0.8631	1303.0	0.6003	682.4
0.2073	0.8685	1315.0	0.6380	665.8
0.0955	0.8705	1328.0	0.6770	651.3
0.0000	0.8718	1339.0	0.7172	639.7
		$T = 313.15$ K		
1.0000	0.7949	1159.1	0.3799	936.4
0.9242	0.8082	1179.3	0.3872	889.6
0.8283	0.8199	1194.0	0.4034	855.5
0.7329	0.8279	1208.3	0.4240	827.2
0.6363	0.8355	1224.0	0.4470	798.9
0.5338	0.8425	1238.0	0.4740	774.4
0.4298	0.8488	1251.0	0.5020	752.8
0.3191	0.8550	1262.0	0.5330	734.3
0.2073	0.8594	1277.0	0.5650	713.6
0.0955	0.8624	1287.6	0.5965	699.4
0.0000	0.8632	1297.5	0.6292	688.2

pressibility, K_S, by using the relation

$$K_S = u^{-2}\rho_m{}^{-1} \qquad (5)$$

The excess isentropic compressibility, K_S^E, was obtained from the relation

$$K_S^E = K_S - K_S^{id} \qquad (6)$$

where K_S is the experimental compressibility and K_S^{id} is

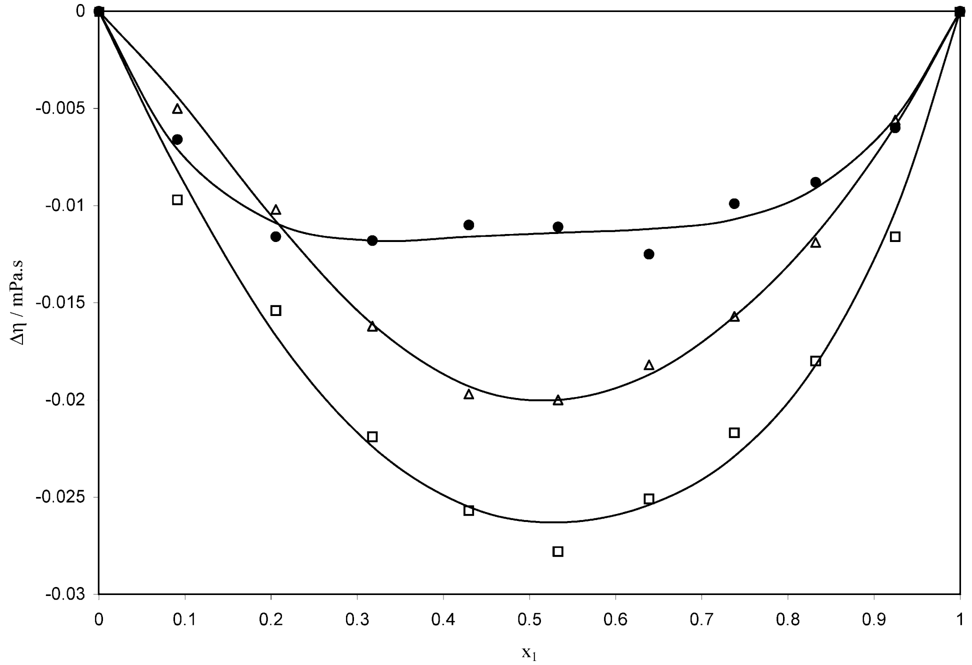

Figure 2. Viscosity deviations, $\Delta\eta$ (mPa·s), for the system 3-pentanone (1) + ethylbenzene (2) at (●) 20 °C, (△) 30 °C, and (□) 40 °C.

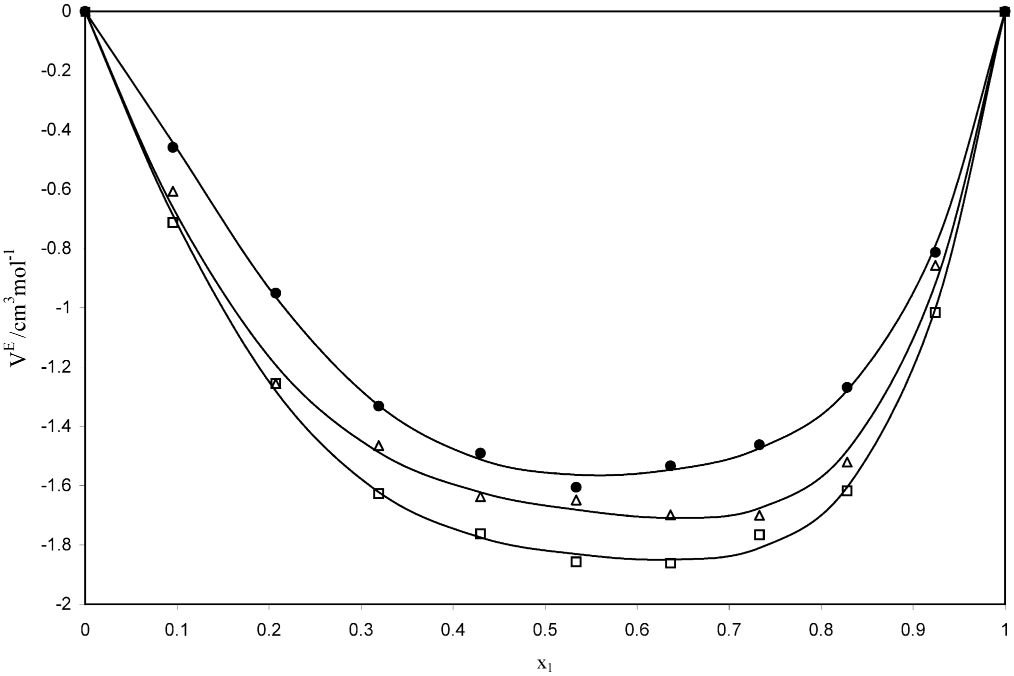

Figure 3. Excess molar volume, V^E (cm^3·mol^{-1}), for the system 3-pentanone (1) + *o*-xylene (2) at (●) 20 °C, (△) 30 °C, and (□) 40 °C.

the isentropic compressibility of an ideal mixture of the components.

K_S^{id} was determined by using Benson's equation[4]

$$K_S^{id} = \sum \phi_i[k^\circ_{S,i} + TV^\circ_i(\alpha^\circ_i)^2/C^\circ_{pi}] - T(\sum x_i V^\circ_i)(\sum \phi_i \alpha^\circ_i)^2/\sum x_i C^\circ_{Pi} \quad (7)$$

where ϕ_i is the volume fraction of i in the mixture stated in terms of the unmixed components, T is the temperature, and $k^\circ_{S,i}$, V°_i, α°_i, and C°_{pi} are the isentropic compressibility, molar volume, coefficient of thermal expansion, and molar heat capacity for pure component i. The values of α were obtained from density values at two different temperatures. The values of molar heat capacity were taken from the literature.[2,5,6]

All the excess properties (V^E and K_S^E) and deviations in viscosity ($\Delta\eta$) were fitted to a Redlich−Kister[7] type equation

$$A = x_1 x_2 \sum_{j=1}^{n} A_{j-1}(x_1 - x_2)^{(j-1)} \quad (8)$$

where A is the property, A_{j-1} is the polynomial coefficient, and n is the polynomial degree.

The standard deviation in each case is calculated using the relation

$$\sigma(X) = \left[\frac{(\sum X_{expt} - X_{calc})^2}{N - n}\right]^{1/2} \quad (9)$$

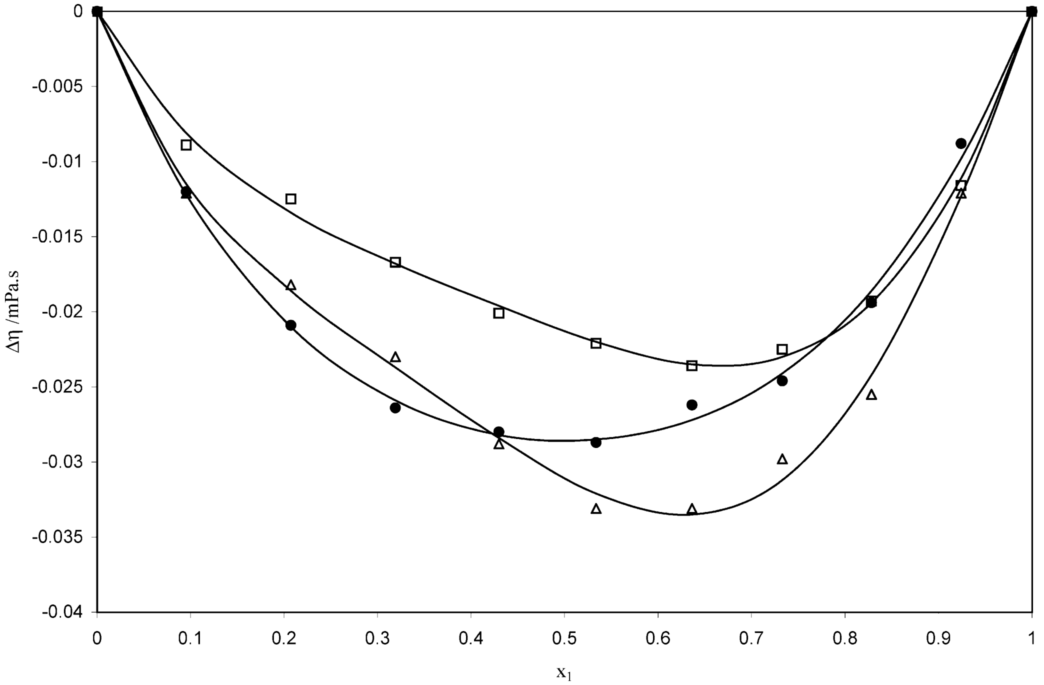

Figure 4. Viscosity deviations, $\Delta\eta$ (mPa·s), for the system 3-pentanone (1) + *o*-xylene (2) at (●) 20 °C, (△) 30 °C, and (□) 40 °C.

Table 4. Values of the Coefficients of the Redlich−Kister Equation (Eq 8) and Standard Deviations (Eq 9)

T/K	A_0	A_1	A_2	A_3	σ
		3-Pentanone (1) + Ethylbenzene (2)			
		V^E/cm^3·mol^{-1}			
293.15	−7.1598	−0.7259	−2.8268	−3.8932	0.0595
303.15	−7.6519	−0.8986	−3.7421	−7.0726	0.0583
313.15	−7.7158	−1.5619	−4.0880	−5.7391	0.0425
		$\Delta\eta$/mPa·s			
293.15	−0.0457	0.0047	−0.0524	0.0016	0.0007
303.15s	−0.0799	−0.0070	0.0171	−0.017	0.0004
313.15	−0.1049	−0.0103	−0.0245	−0.0262	0.0012
		$10^{12}K_S^E$/Pa^{-1}			
293.15	−90.1250	−4.96710	−24.4022	−23.8625	0.6691
303.15	−105.3883	−20.2498	−13.8331	−31.8540	1.0737
313.15	−122.1909	−30.5137	−74.0377	−92.0316	0.9640
		3-Pentanone (1) + *o*-Xylene (2)			
		V^E/cm^3·mol^{-1}			
293.15	−6.2320	−0.6600	−2.6280	−4.2348	0.0231
303.15	−6.6696	−0.9811	−5.2194	−3.0332	0.0457
313.15	−7.2707	−0.8832	−5.3593	−3.9700	0.0257
		$\Delta\eta$/mPa·s			
293.15	−0.1144	−0.0009	−0.0388	−0.0042	0.0007
303.15	−0.1243	−0.0669	−0.0456	0.0615	0.0009
313.15	−0.0852	−0.0447	−0.0584	0.0117	0.0005
		$10^{12}K_S^E$/Pa^{-1}			
293.15	−106.0140	−25.7733	−89.0913	−119.7562	0.9817
303.15	−105.9503	−18.3619	−68.2167	−87.6982	1.1463
313.15	−143.8643	−49.4053	−92.6908	−110.4432	2.0543

where N is the number of data points and n is the number of coefficients.

The values of the coefficients of eq 8 as determined by the method of least squares along with the standard deviations for both the systems are reported in Table 4.

Discussion

The data for both the systems show there is a smooth nonlinear variation of density, viscosity, and ultrasonic velocity with composition over the complete range at all the temperatures. The nonlinear variation of viscosity with composition for the systems is characteristic of systems in which a complex is not formed or in which a complex of low stability occurs. For these systems, the above properties decrease with temperature.

Excess volumes, V^E, (Figures 1 and 3) for the system are negative at all temperatures, and the minimum lies between 0.47 and 0.50 mole fraction of 3-pentanone. The V^E value first decreases, goes to minimum, and again increases with increase in composition of 3-pentanone. With the increase in temperature, the value becomes more and more negative. Deviations in viscosity, $\Delta\eta$, (Figures 2 and 4) are negative over the entire composition range for both the systems. The negative values of the excess volume and $\Delta\eta$ for both the systems indicate the predominance of dipolar forces and the absence of specific interactions.

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