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Densities, Viscosities, and Speed of Sound Studies of Binary Mixtures of Methylbenzene with Heptan-1-ol, Octan-1-ol, and Decan-1-ol at (303.15 and 313.15) K

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Densities, viscosities, and the speed of sound of binary mixtures of methylbenzene with heptan-1-ol, octan-1-ol, and decan-1-ol have been measured over the entire range of composition, at (303.15 and 313.15) K and at atmospheric pressure ($p = 0.1$ MPa). The excess molar volumes (V^E), deviations in viscosity ($\Delta\eta$), and excess isentropic compressibility κ^E_s have been calculated from the experimental values of density, viscosity, and ultrasonic velocity. The excess molar volumes and excess isentropic compressibility are positive for all three binaries studied over the whole composition, whereas deviations in viscosities are negative for all three binary mixtures. The excess molar volumes, deviations in viscosity, and excess isentropic compressibility have been fitted to the Redlich−Kister polynomial equation. The recently proposed Jouyban−Acree model is used to correlate the experimental values of density, viscosity, and ultrasonic velocity at different temperatures.

Introduction

Studies on thermodynamic and transport properties of binary liquid mixtures provide a useful database in a variety of industrial applications. The archival literature provides extensive data on the density and viscosity of liquid mixtures, but a combined study of density, viscosity, and ultrasonic velocity is quite scarce. The volumetric, viscometric, and acoustic properties of binary mixtures containing acetonitrile, dimethylsulfoxide, ethyl acetate, and benzonitrile have been reported earlier.[1−10] Alkanols are self-associated, and there is a decrease in the self-association when they are mixed with methylbenzene as a result of a hydrogen-bonded interaction between the hydroxyl oxygen of alkanols and methylbenzene and because of the presence of a specific interaction between the hydroxyl oxygen of alkanols and the chlorine of methylbenzene. In continuation with our earlier studies of binary mixtures of methylbenzene with alkanols,[11,12] we now report density, viscosity, and ultrasonic velocity data for the binary mixtures for (methylbenzene + heptan-1-ol), (methylbenzene + octan-1-ol), and (methylbenzene + decan-1-ol) at temperatures of (303.15 and 313.15) K.

Experimental Section

Heptan-1-ol, octan-1-ol, decan-1-ol, and methylbenzene (obtained from Qualigens Fine Chemicals, with a mass fraction purity greater than 99.5 mass %) were used after single distillation. Table 1 gives the comparison of experimental values of densities, viscosities, and speed of sound with the corresponding literature values at $T = 303.15$ K. Binary mixtures were prepared by mass in airtight stoppered glass bottles. The masses were recorded on an Adairdutt balance to an uncertainty of $\pm 1 \times 10^{-4}$ g. Care was taken to avoid evaporation and contamination during mixing. The estimated uncertainty in mole fraction was less than 1×10^{-4}.

Table 1. Comparison of Experimental Density, Viscosity, and Ultrasonic Velocity of Pure Liquids with Literature Values at 303.15 K

	$\rho/(\mathrm{g\cdot cm^{-3}})$		$\eta/$ (mPa·s)		$u/(\mathrm{m\cdot s^{-1}})$	
pure liquid	exptl	lit.	exptl	lit.	exptl	lit.
methylbenzene	0.85662	0.85754[a] 0.85660[b]	0.525	0.534[a] 0.526[b]	1289	1285[c]
heptan-1-ol	0.81489	0.81480[d]	5.048	5.030[e]	1313	1313[f]
octan-1-ol	0.81838	0.81752[a] 0.81834[d]	6.433	6.298[e]	1334	1339[d]
decan-1-ol	0.82287	0.82292[d]	9.716		1366	1366[f]

[a] Ref 16. [b] Ref 11. [c] Ref 24. [d] Ref 25. [e] Ref 26f. [f] Ref 27

Densities were determined by using a 15 cm^3 bicapillary pycnometer as described earlier.[9,10] The pycnometer was calibrated using conductivity water with 0.99705 g·cm^{-3} as its density[13] at $T = 298.15$ K. The pycnometer filled with air-bubble-free experimental liquids was kept in a transparent walled water bath in which the temperature was maintained constant to ±0.01 K for between (0.2 and 0.25) h to attain thermal equilibrium. The positions of the liquid levels in the two arms were recorded with the help of a traveling microscope, which could read length to ±0.01 mm. The estimated uncertainty of density measurements of solvent and binary mixtures was 0.000 05 g·cm^{-3}. At least three to four measurements were made which had an average deviation of ±0.000 05 g·cm^{-3}.

The dynamic viscosities were measured using an Ubbelohde suspended level viscometer,[9,10] calibrated with conductivity water having a conductivity of $1 \times 10^{-6}\ \Omega^{-1}\cdot\mathrm{cm}^{-1}$. An electronic digital stopwatch with readability of ±0.01 s was used for the flow time measurements. At least three repetitions of each data reproducible to ±0.05 s were obtained, and the results were averaged. Because all flow times were greater than 200 s and the capillary radius of 0.5 mm was far less than its length of (50 to 60) mm, the kinetic energy and end corrections, respectively, were found to be negligible. The uncertainties in dynamic viscosities are of the order of ±0.003 mPa·s.

The sound speed, u, was measured at a frequency of 2 MHz in these solutions through the interferometric method (using Mittal's F-81 model) at (303.15 and 313.15) K (±0.05 K). No attempt was made to correct the sound speed obtained at a

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Table 2. Density (ρ), Viscosity (η), Ultrasonic Velocity (u), Isentropic Compressibility (κ_s), Excess Molar Volume (V^E), Deviation in Viscosity ($\Delta\eta$), and Excess Isentropic Compressibility (κ_s^E) for Methylbenzene (1) + Alkanols (2) at (303.15 and 313.15) K

x_1	ρ	V^E	η	$\Delta\eta$	u	κ_s	κ_s^E	x_1	ρ	V^E	η	$\Delta\eta$	u	κ_s	κ_s^E
	$g\cdot cm^{-3}$	$cm^3\cdot mol^{-1}$	$mPa\cdot s$	$mPa\cdot s$	$m\cdot s^{-1}$	TPa^{-1}	TPa^{-1}		$g\cdot cm^{-3}$	$cm^3\cdot mol^{-1}$	$mPa\cdot s$	$mPa\cdot s$	$m\cdot s^{-1}$	TPa^{-1}	TPa^{-1}
Methylbenzene (1) + Heptan-1-ol (2) at 303.15 K															
0.0000	0.81489	0.0000	5.048	0.0000	1313	712	0	0.5486	0.83372	0.1650	1.250	−1.3170	1271	742	27
0.0525	0.81652	0.0070	4.404	−0.4070	1310	714	2	0.5903	0.83544	0.1700	1.113	−1.2650	1269	743	28
0.1014	0.81806	0.0170	3.859	−0.7300	1307	716	3	0.6493	0.83795	0.1780	0.982	−1.1290	1266	745	30
0.1518	0.81967	0.0300	3.400	−0.9610	1304	717	4	0.7011	0.84028	0.1760	0.888	−0.9890	1266	743	28
0.1859	0.82078	0.0390	3.154	−1.0530	1301	720	7	0.7520	0.84269	0.1680	0.776	−0.8710	1267	739	24
0.2489	0.82284	0.0630	2.645	−1.2770	1296	724	10	0.8041	0.84527	0.1560	0.673	−0.7380	1268	736	22
0.3011	0.82461	0.0810	2.314	−1.3720	1291	728	14	0.8495	0.84769	0.1310	0.635	−0.5710	1272	729	16
0.3504	0.82634	0.0960	2.042	−1.4210	1286	732	18	0.9009	0.85055	0.0980	0.588	−0.3850	1276	722	11
0.4006	0.82807	0.1230	1.796	−1.4400	1282	735	20	0.9487	0.85339	0.0560	0.546	−0.2110	1282	713	5
0.4494	0.82988	0.1370	1.594	−1.4210	1278	738	23	1.0000	0.85662	0.0000	0.525	0.0000	1289	307	0
0.5003	0.83183	0.1500	1.399	−1.3860	1274	741	26								
Methylbenzene (1) + Heptan-1-ol (2) at 313.15 K															
0.0000	0.80768	0.0000	3.712	0.0000	1279	757	0	0.5486	0.82514	0.2070	1.144	−0.7900	1230	801	36
0.0525	0.80917	0.0160	3.362	−0.1800	1274	761	3	0.5903	0.82672	0.2180	1.069	−0.7300	1227	803	37
0.1014	0.81059	0.0310	3.074	−0.3090	1271	764	5	0.6493	0.82909	0.2230	0.965	−0.6430	1226	802	36
0.1518	0.81207	0.0500	2.770	−0.4500	1267	767	8	0.7011	0.83132	0.2160	0.840	−0.6000	1225	802	36
0.1859	0.81313	0.0570	2.550	−0.5590	1263	771	11	0.7520	0.83357	0.2110	0.772	−0.5030	1226	798	32
0.2489	0.81502	0.0890	2.226	−0.6790	1258	775	14	0.8041	0.83602	0.1950	0.682	−0.4240	1228	793	28
0.3011	0.81669	0.1060	1.986	−0.7500	1251	782	20	0.8495	0.83832	0.1670	0.639	−0.3200	1232	786	22
0.3504	0.81824	0.1330	1.770	−0.8060	1247	786	23	0.9009	0.84107	0.1270	0.573	−0.2190	1239	775	14
0.4006	0.81987	0.1590	1.583	−0.8310	1242	791	28	0.9487	0.84385	0.0720	0.528	−0.1090	1245	765	8
0.4494	0.82157	0.1730	1.436	−0.8190	1237	795	31	1.0000	0.84703	0.0000	0.471	0.0000	1256	748	0
0.5003	0.82335	0.1950	1.271	−0.8200	1233	799	34								
Methylbenzene (1) + Octan-1-ol (2) at 303.15 K															
0.0000	0.81838	0.000	6.433	0.000	1334	687	0	0.5513	0.83446	0.196	1.541	−1.635	1276	736	34
0.0495	0.81962	0.011	5.630	−0.511	1329	691	3	0.6014	0.83631	0.209	1.350	−1.530	1272	739	35
0.1104	0.82119	0.027	4.775	−1.006	1325	694	4	0.6495	0.83822	0.211	1.214	−1.382	1270	740	35
0.1513	0.82225	0.044	4.281	−1.258	1321	697	6	0.6997	0.84036	0.204	1.065	−1.234	1268	740	34
0.1999	0.82355	0.063	3.788	−1.464	1316	701	9	0.7569	0.84290	0.198	0.931	−1.030	1267	739	31
0.2517	0.82498	0.084	3.280	−1.666	1310	706	12	0.8012	0.84502	0.184	0.819	−0.881	1268	736	28
0.2997	0.82634	0.106	2.952	−1.710	1304	712	17	0.8527	0.84770	0.153	0.733	−0.662	1269	733	24
0.3560	0.82802	0.128	2.504	−1.826	1297	718	21	0.9000	0.85032	0.118	0.646	−0.470	1273	726	17
0.3998	0.82932	0.154	2.229	−1.842	1291	724	26	0.9540	0.85360	0.060	0.576	−0.221	1280	715	8
0.4506	0.83099	0.166	1.974	−1.797	1286	728	29	1.0000	0.85662	0.000	0.525	0.000	1289	703	0
0.5001	0.83263	0.186	1.758	−1.720	1281	732	31								
Methylbenzene (1) + Octan-1-ol (2) at 313.15 K															
0.0000	0.81105	0.000	4.603	0.000	1304	725	0	0.5513	0.82577	0.257	1.175	−1.150	1238	790	46
0.0495	0.81214	0.026	4.130	−0.268	1300	729	3	0.6014	0.82751	0.268	1.084	−1.034	1234	794	48
0.1104	0.81356	0.053	3.645	−0.502	1293	735	7	0.6495	0.82930	0.270	0.935	−0.984	1231	796	49
0.1513	0.81455	0.070	3.261	−0.717	1287	741	11	0.6997	0.83129	0.265	0.866	−0.846	1228	798	49
0.1999	0.81573	0.096	2.832	−0.945	1282	746	15	0.7569	0.83369	0.255	0.754	−0.721	1228	795	44
0.2517	0.81704	0.123	2.545	−1.018	1274	754	21	0.8012	0.83574	0.233	0.703	−0.589	1229	792	40
0.2997	0.81829	0.148	2.218	−1.147	1268	760	25	0.8527	0.83828	0.198	0.636	−0.444	1232	786	33
0.3560	0.81985	0.172	1.944	−1.188	1262	766	29	0.9000	0.84085	0.149	0.558	−0.326	1236	779	25
0.3998	0.82103	0.204	1.715	−1.236	1255	773	35	0.9540	0.84400	0.084	0.526	−0.135	1245	764	12
0.4506	0.82256	0.222	1.518	−1.223	1250	778	38	1.0000	0.84703	0.000	0.471	0.000	1256	748	0
0.5001	0.82408	0.244	1.370	−1.167	1242	787	45								
Methylbenzene (1) + Decan-1-ol (2) at 303.15 K															
0.0000	0.82287	0.000	9.716	0.000	1366	651	0	0.5497	0.83529	0.220	2.152	−2.520	1290	719	40
0.0507	0.82376	0.020	8.474	−0.777	1361	655	2	0.6009	0.83692	0.230	1.883	−2.320	1285	724	41
0.1015	0.82473	0.032	7.424	−1.361	1355	660	5	0.6498	0.83861	0.235	1.594	−2.160	1280	728	42
0.1473	0.82562	0.048	6.635	−1.730	1349	666	9	0.7065	0.84080	0.224	1.414	−1.820	1275	732	42
0.2091	0.82688	0.070	5.658	−2.140	1340	674	14	0.7524	0.84270	0.214	1.150	−1.662	1274	731	38
0.2577	0.82790	0.093	4.962	−2.390	1333	680	17	0.8069	0.84515	0.197	1.021	−1.291	1273	730	33
0.3006	0.82884	0.113	4.458	−2.500	1327	685	20	0.8472	0.84718	0.171	0.887	−1.056	1274	727	27
0.3496	0.82995	0.139	3.848	−2.660	1318	694	27	0.9063	0.85054	0.110	0.750	−0.650	1278	720	17
0.4028	0.83122	0.168	3.320	−2.700	1311	700	30	0.9489	0.85312	0.070	0.599	−0.410	1282	713	8
0.4516	0.83248	0.189	2.843	−2.730	1303	708	35	1.0000	0.85662	0.000	0.525	0.000	1289	703	0
0.4989	0.83377	0.208	2.499	−2.640	1295	715	39								
Methylbenzene (1) + Decan-1-ol (2) at 313.15 K															
0.0000	0.81597	0.000	6.820	0.000	1334	689	0	0.5497	0.82706	0.270	1.470	−1.860	1255	768	47
0.0507	0.81674	0.031	6.060	−0.438	1327	695	4	0.6009	0.82857	0.277	1.305	−1.700	1249	774	50
0.1015	0.81758	0.054	5.343	−0.833	1320	702	8	0.6498	0.83011	0.281	1.162	−1.532	1245	777	49
0.1473	0.81834	0.082	4.771	−1.114	1314	708	12	0.7065	0.83212	0.270	0.994	−1.340	1240	782	49
0.2091	0.81945	0.113	4.059	−1.433	1305	717	18	0.7524	0.83386	0.260	0.905	−1.138	1239	781	45
0.2577	0.82038	0.135	3.552	−1.632	1297	725	23	0.8069	0.83621	0.227	0.790	−0.907	1239	779	38
0.3006	0.8212	0.163	3.112	−1.800	1292	730	26	0.8472	0.83804	0.207	0.732	−0.709	1240	776	32
0.3496	0.82224	0.183	2.710	−1.890	1283	739	32	0.9063	0.84118	0.140	0.640	−0.426	1243	769	21
0.4028	0.82338	0.214	2.263	−2.000	1275	747	36	0.9489	0.84358	0.097	0.565	−0.230	1248	761	11
0.4516	0.82449	0.242	1.903	−2.050	1268	754	40	1.0000	0.84703	0.000	0.471	0.000	1256	748	0
0.4989	0.82569	0.256	1.678	−1.975	1261	762	45								

Table 3. Parameters and Standard Deviations (σ) of Eqs 5 and 6 for Methylbenzene + Heptan-1-ol, Methylbenzene + Octan-1-ol, and Methylbenzene + Decan-1-ol

	T/K	a_0	a_1	a_2	a_3	σ
		Methylbenzene + Heptan-1-ol				
V^E/(cm^3·mol^{-1})	303.15	0.606	0.570	0.051		0.002
	313.15	0.765	0.663	0.164		0.003
$\Delta\eta$/(mPa·s)	303.15	−5.5170	2.1466	−0.927		0.014
	313.15	−3.262	0.9615	0.4426	−0.370	0.012
κ^E_s/(TPa^{-1})	303.15	104.183	99.126	−41.559	−74.000	0.817
	313.15	135.488	107.044	−35.307	−62.075	0.626
		Methylbenzene + Octan-1-ol				
V^E/(cm^3·mol^{-1})	303.15	0.738	0.611	0.077	0.034	0.002
	313.15	0.949	0.7247	0.2786		0.004
$\Delta\eta$/(mPa·s)	303.15	−6.908	3.0573	−1.2987	0.2225	0.016
	313.15	−4.797	1.7187	0.4918	−0.5634	0.025
κ^E_s/(TPa^{-1})	303.15	123.201	119.960	−8.025	−56.296	1.035
	313.15	173.602	143.199	−2.853	−30.493	0.8519
		Methylbenzene + Decan-1-ol				
V^E/(cm^3·mol^{-1})	303.15	0.810	0.736	0.081	−0.203	0.004
	313.15	0.996	0.690	0.291		0.006
$\Delta\eta$/(mPa·s)	303.15	−10.324	3.611	−1.834	0.997	0.046
	313.15	−7.739	2.473	1.092		0.029
κ^E_s/(TPa^{-1})	303.15	154.682	138.070	−43.876	−83.363	1.101
	313.15	181.179	144.020	−24.632	−75.759	0.828

frequency to the zero frequency thermodynamic value. The estimated error in sound speed measurements is ±1 m·s^{-1}. The other experimental details are the same as those reported earlier.[9,10]

Results and Discussion

Experimental values of densities (ρ), viscosities (η), and ultrasonic velocities (u) of mixtures at temperatures of (303.15 and 313.15) K are listed as a function of mole fraction in Table 2. The density values have been used to calculate excess molar volumes (V^E) using the following equation

$$V^E/\text{cm}^3\cdot\text{mol}^{-1} = (x_1M_1 + x_2M_2)/\rho_{12} - (x_1M_1/\rho_1) - (x_2M_2/\rho_2) \quad (1)$$

where ρ_{12} is the density of the mixture and x_1, M_1, ρ_1 and x_2, M_2, ρ_2 are the mole fraction, the molecular weight, and the density of pure components 1 and 2, respectively.

The viscosity deviations $\Delta\eta$ were calculated using

$$\Delta\eta/\text{mPa}\cdot\text{s} = \eta_{12} - x_1\eta_1 - x_2\eta_2 \quad (2)$$

where η_{12} is the viscosity of the mixture and x_1, x_2 and η_1, η_2 are the mole fraction and the viscosity of pure components 1 and 2, respectively.

The excess isentropic compressibility, κ_s^E, was obtained using the relation

$$\kappa_s^E = \kappa_s - \kappa_s^{id} \quad (3)$$

where κ_s is the isentropic compressibility and was calculated using the Laplace relation; that is, $\kappa_s = (1/u^2\rho)$ and κ_s^{id} were calculated from the relation[14,15]

$$\kappa_s^{id} = \Sigma\phi_i[\kappa_{s,i} + TV^o_i(\alpha^{o\,2}_i)/C_{p,i}] - [T(\Sigma x_iV^o_i)(\Sigma\phi_i\alpha^o_i)^2/\Sigma x_iC_{p,i}] \quad (4)$$

where ϕ_i is the volume fraction of the component i in the mixture stated, T is the temperature, and $\kappa_{s,i}$, V^o_i, α^o_i, and $C_{p,i}$ are the isentropic compressibility, molar volume, coefficient of thermal expansion, and molar heat capacity, respectively, for pure component i. The values required were taken from the literature.[16,17]

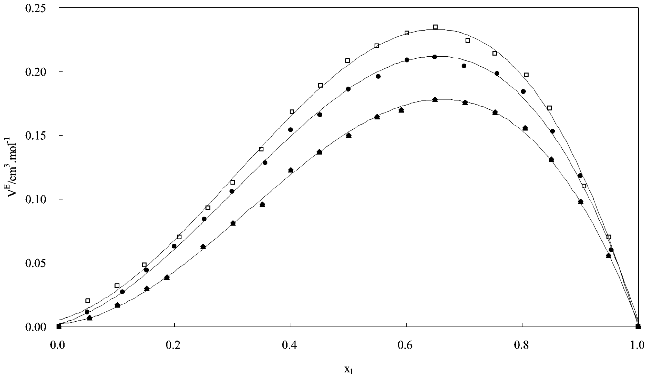

Figure 1. Excess molar volumes V^E at 303.15 K for x_1 methylbenzene + (1 − x_1) alkanols: ▲, pentan-1-ol; ●, octan-1-ol; □, decan-1-ol.

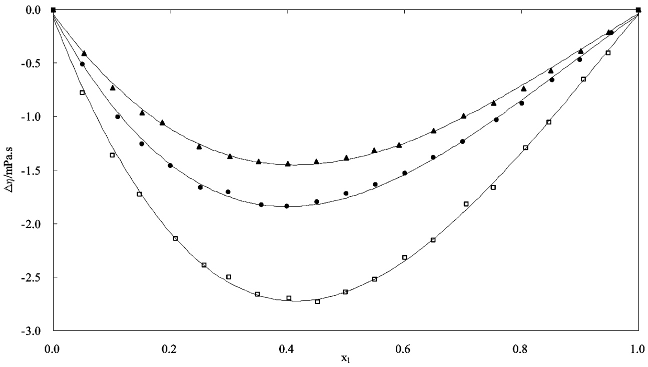

Figure 2. Deviations in viscosity ($\Delta\eta$) at 303.15 K for x_1 methylbenzene + (1 − x_1) alkanols: ▲, pentan-1-ol; ●, octan-1-ol; □, decan-1-ol.

The excess molar volumes and deviations in viscosity and isentropic compressibility were fitted to the Redlich−Kister[18] equation of the type

$$Y = x_1x_2\sum_i^n a_i(x_1 - x_2)^i \quad (5)$$

where Y is either V^E, $\Delta\eta$, or κ_s^E and n is the degree of polynomial. Coefficients a_i were obtained by fitting eq 5 to experimental results using a least-squares regression method. In each case, the optimum number of coefficients is ascertained from an examination of the variation in standard deviation (σ).

σ was calculated using the relation

$$\sigma(Y) = \left[\frac{\sum(Y_{\text{exptl}} - Y_{\text{calcd}})^2}{N - n}\right]^{1/2} \quad (6)$$

where N is the number of data points and n is the number of coefficients. The calculated values of the coefficients (a_i) along with the standard deviations (σ) are given in Table 3.

The variation of V^E with the mole fraction x_1 of methylbenzene for heptan-1-ol, octan-1-ol, and decan-1-ol at 303.15 K is represented in Figure 1. The observed positive excess molar volumes in the present investigation may be discussed in terms of several effects.[19] The mixtures of methylbenzene with alkanols show the trend heptan-1-ol < octan-1-ol < decan-1ol.

Figure 2 depicts the variation of $\Delta\eta$ with the mole fraction x_1 of methylbenzene. $\Delta\eta$ values are negative in all systems and become more negative with an increase in chain length of alkanols, suggesting a decrease in hetero association of molecules with an increase in molar mass of alkanols.

McAllister's multibody interaction models[20] have been used to correlate the kinematic viscosities of binary liquid mixtures.

Table 4. Correlated Results of McAllister's Multibody Models.

		three−body model			four−body model			
mixture	T/K	ν_{12}	ν_{21}	σ	ν_{1112}	ν_{1122}	ν_{2221}	σ
methylbenzene+	303.15	0.868	2.749	2.05	0.738	1.661	3.120	0.07
heptan-1-ol	313.15	1.078	2.352	1.60	0.974	1.210	2.962	0.05
methylbenzene+	303.15	1.289	3.228	1.06	1.039	1.852	3.900	0.05
octan-1-ol	313.15	1.047	2.610	2.06	0.971	1.132	3.442	0.08
methylbenzene+	303.15	1.822	5.157	2.36	1.430	2.541	5.992	0.13
decan-1-ol	313.15	1.477	3.459	5.04	1.407	1.050	5.234	0.13

The three-body McAllister model is defined by

$$\ln \nu = x_1^3 \ln \nu_1 + x_2^3 \ln \nu_2 + 3x_1^2x_2 \ln \nu_{12} + 3x_1x_2^2 \ln \nu_{21} - \ln[x_1 + (x_2M_2/M_1)] + 3x_1^2x_2 \ln[(2/3) + (M_2/3M_1)] + 3x_1x_2^2 \ln[(1/3) + (2M_2/3M_1)] + x_2^3 \ln(M_2/M_1) \quad (7)$$

and the four-body McAllister model is defined by

$$\ln \nu = x_1^4 \ln \nu_1 + 4x_1^3x_2 \ln \nu_{1112} + 6x_1^2x_2^2 \ln \nu_{1122} + 4x_1x_2^3 \ln \nu_{2221} + x_2^4 \ln \nu_2 - \ln[x_1 + (x_2M_2/M_1)] + 4x_1^3x_2 \ln[\{3 + (M_2/M_1)\}/4] + 6x_1^2x_2^2 \ln[\{1 + (M_2/M_1)\}/2] + 4x_1x_2^3 \ln[\{(1 + 3M_2/M_1)\}/4] + x_2^4 \ln(M_2/M_1) \quad (8)$$

where ν_{12}, ν_{21}, ν_{1122}, ν_{1122}, and ν_{2221} are interaction parameters and M_1 and M_2 are molecular weights of components 1 and 2.

The correlating ability of eqs 7 and 8 was tested by calculating the percentage standard deviation (σ %) between the experimental and calculated viscosity as

$$\sigma\,\% = [1/(n - m)\Sigma\{(100(\nu_{\text{exptl}} - \nu_{\text{calcd}})/\nu_{\text{exptl}})^2\}^{1/2}] \quad (9)$$

where n represents the number of experimental points and m represents the number of coefficients. Table 4 includes the different parameters for McAllister's three-body and four-body models. From Table 4, it is clear that McAllister's four-body interaction model gives a better result than the three-body model for correlating the kinematic viscosities of the binary mixtures studied.

The variation of κ^E_s with the mole fraction of methylbenzene, x_1, is represented in Figure 3. Kiyohara and Benson[21] have suggested that κ^E_s is the resultant of several opposing effects. The mixtures of methylbenzene with alkanols show the trend heptan-1-ol < octan-1-ol < decan-1ol.

Recently, Jouyban et al.[22,23] proposed a model for correlating the density and viscosity of liquid mixtures at various temperatures (the Jouyban−Acree model). The proposed equation is

$$\ln y_{m,T} = f_1 \ln y_{1,T} + f_2 \ln y_{2,T} + f_1f_2\Sigma[A_j(f_1 - f_2)^j/T] \quad (10)$$

where $y_{m,T}$, $y_{1,T}$, and $y_{2,T}$ are density or viscosity of the mixture and solvents 1 and 2 at temperature T, respectively, $f_1$and f_2 are the volume fractions of solvents in the case of density and the mole fractions in the case of viscosity, and A_j is the model constant.

The correlating ability of the Jouyban−Acree model was tested by calculating the average percentage deviation (APD) between the experimental and calculated density and viscosity as

$$\text{APD} = (1/N)\Sigma[(|y_{\text{exptl}} - y_{\text{calcd}}|)/y_{\text{exptl}}] \quad (11)$$

where N is the number of data points in each set. The optimum numbers of constants (A_j), in each case, were determined from the examination of the average percentage deviation value.

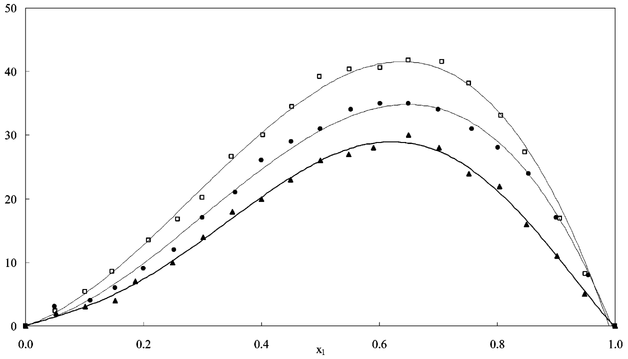

Figure 3. Excess isentropic compressibility (κ^E_s) at 303.15 K for x_1 alkanols: ▲, pentan-1-ol; ●, octan-1-ol; □, decan-1-ol.

Table 5. Parameters of the Jouyban−Acree Model and Average Percentage Deviation for Densities, Viscosities, and Ultrasonic Velocities at (303.15 and 313.15) K

system	A_o	A_1	A_2	APD
Density				
methylbenzene + pentan-1-ol	−5.531	−2.291	−0.573	0.011
methylbenzene + octan-1-ol	−6.952	−2.964	−0.991	0.014
methylbenzene + decan-1-ol	−8.384	−3.885	−1.485	0.006
Viscosity				
methylbenzene + pentan-1-ol	−29.611	−22.821	−1.601	5.318
methylbenzene + octan-1-ol	−68.312	−51.31	38.873	1.534
methylbenzene + decan-1-ol	38.223	17.788	134.413	3.975
Ultrasonic Velocity				
methylbenzene + pentan-1-ol	−29.611	−22.821	−1.601	0.256
methylbenzene + octan-1-ol	−31.818	−30.161	−7.291	0.222
methylbenzene + decan-1-ol	−30.412	−27.179	−3.290	0.126

The Jouyban−Acree model was not previously applied to ultrasonic velocity measurements. We extend the Jouyban−Acree model (eq 10) to the ultrasonic velocity of the liquid mixtures with f as the mole fraction and again apply eq 11 for the correlating ability of the model.

The constants A_j calculated from the least-squares analysis are presented in Table 5 along with the average percentage deviation (APD). The proposed model provides reasonably accurate calculations for the density, viscosity, and ultrasonic velocity of binary liquid mixtures at various temperatures, and the model could be used in data modeling.

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