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Study of molecular interactions in binary liquid mixtures containing tri-*n*-butylamine with 2-pentanone, 3-pentanone, and 4-methyl-2-pentanone: A thermophysical approach

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ABSTRACT

This paper reports experimental densities (ρ) and speeds of sound (u) of tri-*n*-butyl amine (TBA), 2-pentanone (2P), 3-pentanone (3P), 4-methyl-2-pentanone (4M2P) and their binary mixtures with TBA as common component, measured at atmospheric pressure and T = (293.15, 298.12, 303.15, 308.15 and 313.15) K over the entire composition range. Experimental viscosities (η) under similar condition of composition and pressure are also reported at T = (298.15, 303.15, and 308.15) K. Excess molar volumes (V_m^E), excess isentropic compressibility ($\Delta\kappa_s$) and deviations in speed of sound (Δu) of all the binary mixtures were evaluated from the experimental results of density and speed of sound data. All these thermodynamic properties are analyzed in terms of intermolecular interactions and structural effects present between the molecules of the investigated binary liquid mixtures. Further, viscosity data were used to calculate deviations in viscosity ($\Delta\eta$) and excess Gibb's free energy of activation for viscous flow (ΔG^{*E}). The derived properties have also been correlated to composition using Redlich–Kister type polynomial equation by the method of least-square for the estimation of the binary coefficients and the standard errors. Apart from this, various semi empirical relations i.e. Grunberg–Nissan, Tamura–Kurata, Katti–Chaudhri, McAllister (3-body interaction) and Heric-Brewer (3-parameter) have been tested using experimental viscosity data.

1. Introduction

Binary liquid mixtures are very important from the industry point of view, because they provide a wide range of mixtures with desired properties and can be used as solvents in many chemical, industrial and biological processes. Further, viscosity is also used for hydraulic calculations, transport of fluid, mass and energy in industry [1]. Thermophysical properties derived from density, speed of sound and viscosity data on binary liquid mixtures are consecutive source for characterization of intermolecular interactions and structural arrangements between the molecules of liquid components and for the development of molecular models [2]. The understanding of these properties on binary mixtures is also helpful to design processes [3]. In biochemistry, molecules containing >NH_2 and >C═O groups are used as simple models because these functional groups are very common in nature e.g. proteins and peptides [4]. Further, molecules containing these functional groups are also very important from the industry point of view e.g. caprolactam is used for the preparation of nylon-6. After going through an exhaustive literature survey it has been found that there is lack of data on the liquid mixtures containing aliphatic amine and aliphatic ketone as very few research groups [5–9] are working on it. Keeping in view the wide applications of >NH_2 and >C═O groups, our present investigation focuses on the study of thermophysical properties of binary liquid mixtures of amine with ketones.

Table 1
Provenance and purity[a] of chemicals used.

Sr. no.	Chemical name	Provenance	Mass fraction purity[a]
1	Tri-*n*-butyl amine	S. D. Fine Chemicals Ltd.	>0.99
2	2-Pentanone	HiMedia Labs. Pvt. Ltd.	>0.99
3	3-Pentanone	HiMedia Labs. Pvt. Ltd	>0.99
4	4-Methyl-2-pentanone	S. D. Fine Chemicals Ltd	>0.99

[a] as stated by the manufacturer.

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Table 2
Comparison of experimental and literature values of density (ρ) and viscosity (η) of used pure liquids at different temperatures and at atmospheric pressure.

Name of chemical	Temperature/K	$\rho \times 10^{-3}$/kg·m^{-3}		η/mPa·s	
		Exp.	Lit.	Exp.	Lit.
Tri-*n*-butyl amine	298.15	0.77320	0.77318 [12]	1.273	1.258 [13]
	303.15	0.76946	0.7692 [14]	1.157	1.1670 [15]
	308.15	0.76572	0.7657 [14]	1.064	1.028 [14]
2-Pentanone	298.15	0.80282	0.8021 [16]	0.463	0.469 [17]
	303.15	0.79793	0.7975 [18]	0.437	0.435 [19]
	308.15	0.79301	0.79325 [19]	0.413	–
3-Pentanone	298.15	0.80968	0.80977 [20]	0.437	0.440 [21]
	303.15	0.80477	0.8047 [22]	0.414	0.4231 [22]
	308.15	0.79984	0.8000 [23]	0.393	0.397 [24]
4-Methyl-2-pentanone	298.15	0.79621	0.7959 [25]	0.540	0.54663 [26]
	303.15	0.79161	0.79193 [27]	0.505	–
	308.15	0.78698	0.7877 [28]	0.476	–

Table 3
Density (ρ) and speed of sound (u) for the mixtures over entire composition range containing tri-*n*-butylamine and ketones at studied temperatures and atmospheric pressure.

x_1	$\rho \times 10^{-3}$/(kg m^{-3})					u/(m s^{-1})				
	293.15	298.15	303.15	308.15	313.15	293.15	298.15	303.15	308.15	313.15
Tri-*n*-butylamine + 2-pentanone										
0	0.80768	0.80282	0.79793	0.79301	0.78808	1235.74	1214.79	1194.35	1174.33	1154.14
0.0499	0.80323	0.79902	0.79351	0.78872	0.78392	1235.41	1214.79	1194.07	1171.41	1150.95
0.1000	0.79965	0.79494	0.79023	0.78560	0.78084	1236.10	1215.34	1194.20	1170.20	1149.53
0.1499	0.79652	0.79194	0.78733	0.78271	0.77807	1235.96	1215.42	1196.47	1172.69	1152.52
0.2000	0.79377	0.78927	0.78475	0.78022	0.77567	1234.90	1214.42	1193.57	1172.53	1151.28
0.2498	0.79149	0.78706	0.78262	0.77816	0.77369	1233.28	1213.14	1193.25	1172.94	1151.99
0.3000	0.78960	0.78523	0.78086	0.77646	0.77206	1233.06	1213.14	1193.15	1173.31	1152.86
0.3999	0.78628	0.78203	0.77777	0.77350	0.76923	1235.78	1215.75	1195.88	1175.98	1156.12
0.4997	0.78374	0.77960	0.77544	0.77128	0.76711	1238.91	1219.13	1199.56	1179.92	1160.28
0.5997	0.78170	0.77764	0.77359	0.76952	0.76545	1243.72	1224.02	1204.46	1184.91	1165.35
0.7002	0.78006	0.77611	0.77214	0.76817	0.76418	1248.89	1228.49	1209.05	1189.72	1170.49
0.7997	0.77874	0.77485	0.77098	0.76709	0.76319	1252.71	1233.44	1214.41	1194.98	1175.43
0.8463	0.77824	0.77440	0.77054	0.76670	0.76284	1254.26	1235.11	1215.98	1196.92	1178.26
0.8990	0.77778	0.77398	0.77016	0.76634	0.76253	1256.54	1237.69	1218.71	1199.94	1181.23
0.9560	0.77727	0.77351	0.76973	0.76596	0.76218	1260.05	1240.55	1221.56	1203.09	1184.53
1	0.77693	0.77320	0.76946	0.76572	0.76197	1261.76	1242.80	1224.04	1205.49	1187.17
Tri-*n*-butylamine + 3-pentanone										
0	0.81458	0.80968	0.80477	0.79984	0.79489	1236.92	1216.31	1195.83	1175.28	1155.24
0.0500	0.81000	0.80520	0.80036	0.79553	0.79072	1237.08	1216.80	1197.03	1175.64	1154.41
0.1004	0.80586	0.80116	0.79645	0.79172	0.78698	1237.54	1217.55	1197.33	1175.11	1154.46
0.1502	0.80242	0.79781	0.79319	0.78854	0.78389	1237.57	1217.72	1197.90	1175.39	1155.47
0.2006	0.79932	0.79478	0.79024	0.78568	0.78110	1237.12	1216.95	1196.83	1176.60	1155.95
0.2500	0.79670	0.79223	0.78776	0.78327	0.77878	1237.23	1217.02	1196.93	1176.92	1156.75
0.2996	0.79429	0.78985	0.78541	0.78101	0.77657	1238.20	1218.17	1198.31	1177.92	1158.01
0.3995	0.78984	0.78558	0.78131	0.77703	0.77274	1240.43	1220.45	1200.55	1180.60	1160.94
0.4998	0.78646	0.78231	0.77815	0.77398	0.76981	1243.13	1223.26	1203.51	1183.79	1164.44
0.6004	0.78381	0.77976	0.77570	0.77163	0.76755	1246.02	1226.32	1206.73	1187.32	1168.19
0.7005	0.78160	0.77764	0.77367	0.76969	0.76570	1249.51	1230.00	1210.66	1191.44	1172.46
0.7998	0.77979	0.77590	0.77201	0.76811	0.76421	1253.21	1233.81	1214.56	1195.45	1176.77
0.8462	0.77905	0.77520	0.77135	0.76748	0.76361	1255.47	1235.98	1216.55	1197.57	1179.10
0.8953	0.77843	0.77461	0.77080	0.76696	0.76311	1257.16	1238.01	1218.40	1199.52	1181.64
0.9489	0.77776	0.77399	0.77022	0.76643	0.76264	1258.33	1239.75	1220.48	1201.47	1183.71
1	0.77693	0.77320	0.76946	0.76572	0.76197	1261.76	1242.80	1224.04	1205.49	1187.17
Tri-*n*-butylamine + 4-methyl-2-pentanone										
0	0.80080	0.79621	0.79161	0.78698	0.78235	1208.94	1188.88	1168.88	1148.89	1128.96
0.0501	0.79800	0.79348	0.78894	0.78438	0.77982	1210.06	1189.99	1169.94	1150.10	1130.35
0.1000	0.79562	0.79116	0.78669	0.78220	0.77769	1212.13	1192.07	1172.20	1152.35	1132.66
0.1499	0.79341	0.78900	0.78459	0.78015	0.77571	1214.16	1194.10	1174.25	1154.47	1134.93
0.2004	0.79159	0.78724	0.78288	0.77850	0.77410	1217.25	1197.34	1177.73	1158.05	1138.11
0.2500	0.78985	0.78556	0.78125	0.77692	0.77258	1220.49	1200.30	1180.77	1160.96	1140.79
0.3017	0.78824	0.78399	0.77973	0.77546	0.77117	1222.77	1203.05	1183.51	1163.68	1143.52
0.4004	0.78561	0.78146	0.77728	0.77310	0.76891	1227.25	1207.61	1188.11	1168.73	1149.03
0.4999	0.78340	0.77933	0.77524	0.77114	0.76703	1232.92	1213.32	1193.88	1174.26	1154.86
0.6004	0.78165	0.77765	0.77363	0.76961	0.76559	1237.97	1218.47	1199.12	1179.85	1160.77
0.6962	0.78017	0.77624	0.77230	0.76835	0.76440	1243.16	1223.76	1204.53	1185.41	1166.68
0.8004	0.77887	0.77502	0.77115	0.76728	0.76340	1249.12	1229.87	1210.80	1191.92	1173.44
0.8496	0.77848	0.77465	0.77082	0.76697	0.76313	1251.62	1232.38	1213.83	1194.97	1176.48
0.8997	0.77812	0.77431	0.77050	0.76668	0.76286	1255.33	1236.21	1217.24	1198.46	1180.01
0.9499	0.77776	0.77398	0.77019	0.76640	0.76261	1258.52	1239.79	1220.61	1201.90	1183.42
1	0.77693	0.77320	0.76946	0.76572	0.76197	1261.76	1242.80	1224.04	1205.49	1187.17