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Theoretical evaluation of ultrasonic velocity in binary mixtures of isomeric butanols with ethyl benzoate

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ABSTRACT

Theoretical values of ultrasonic velocity in binary liquid mixtures of ethyl benzoate + 2- methyl -1- propanol, ethyl benzoate + 2-butanol and ethyl benzoate + 2- methyl -2- propanol have been evaluated at 303.15,308.15,313.15 and 318.15K using Nomoto's relation, ideal mixing relation (IMR) impedance dependence relation (IDR), Rao's velocity method (RVM) and Junjie's method (JM). The relative merits of these theoretical relations were examined by comparing the theoretical values of ultrasonic velocity with the values obtained experimentally. The validity of the theories was checked by applying the chi-square test for goodness of fit and by calculating the average percentage error (APE).

Keywords: Ultrasonic Velocity, ethyl benzoate, Alcohols, Chi-Square Test

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INTRODUCTION

In recent years measurement of ultrasonic investigations found wide applications in determining the Physicochemical behavior of liquid mixtures [1–5]. Many researchers [6–9] carried out ultrasonic investigations and correlated the experimental results of ultrasonic velocity with the theoretical relations of Nomoto [10, 11], Van Deal and Vangeel ideal mix relations [12] impedance relation [13] Rao's Specific velocity [14] and Junjie [15] and interpreted the results in terms of molecular interactions.

Sound velocity in a liquid is discussed by Longeman and Correy [16] as the sum of bond velocities .Rendall [17] has shown a close agreement between the experimental and theoretical values calculated from the adiabatic compressibility measurements. Auslander and Onitni [18], Samal and Misra [19], Aziz et al. [20,21], and Younglove [22] showed that there is close relation between sound velocity and thermodynamic properties.

In the present investigation ethyl benzoate is mixed with alcohols at different mole fractions to study the interactions between the component molecules. The results are explained and discussed in terms of molecular interactions present in the investigated systems.

The deviation in the variation of U^2_{exp}/ U^2_{imx}, average percentage error, (APE), Chi-square test for goodness of fit, from unity have also been evaluated to further explain the non-ideality of the system. The ratio of $U_{exp}{}^{2/}U_{imx}{}^{2}$ gives an idea of extent of interaction taking place between molecules of the mixtures, positive values of which infer strong interactions between the components.

MATERIALS AND METHODS

Ethyl benzoate , 2- methyl -1- propanol, 2-butanol and 2- methyl- 2- propanol from Merk were purified as described

in the literature [23,24]. The pure chemicals were stored over activated 4Å molecular sieves to reduce water content before use.

The mixtures are prepared gravimetrically using an electronic balance (Shimadzu AY120) with an uncertainty of $\pm 1x10^{-7}$kg and stored in airtight bottles. The uncertainty on mole fraction is estimated to be $1x10^{-4}$.It is ensured that the mixtures are properly mixed and the measurement of the required parameters was done within one day of preparation.

The densities, ρ, of pure liquids and their mixtures are determined using a 10^{-5} m^3 double-arm pycnometer, and the values from triplicate replication at each temperature are reproducible within 2 x 10^{-1} kg m^3 and the uncertainty in the measurement of density is found to be 2 parts in 10^4 parts. The reproducibility in mole fractions was within ±0.0002

Temperature control for the measurement of viscosity and density is achieved by using a microprocessor assisted circulating water bath, (supplied by Mac, New Delhi) regulated to ±0.01 K, using a proportional temperature controller. Adequate precautions were taken to minimize evaporation losses during the actual measurements.
The ultrasonic velocity of sound (U) is measured using an ultrasonic interferometer (Mittal Enterprises, New Delhi model F05) operating at 2 MHz The measured speeds of sound have a precision of 0.8 $m.sec^{-1}$ and an uncertainty less than ± 0.1 $m.sec^{-1}$. The temperature stability was maintained within±0.01K.by circulating water bath around the measuring cell through a pump.

THEORETICAL CONIDERATIONS

Nomoto Equation

Rao [14] proposed the relation that the ratio of temperature coefficients of sound velocity U and molar volume V remains almost constant for pure liquids:

$$[(1/U)\,(dU/dT)] / [(1/V)\,(dV/dT)] = -3 \qquad (1)$$

where T is the absolute temperature.

Integration the above equation, we get

$$VU^{1/3} = \text{const} = M/\rho U^{1/3} = R \qquad (2)$$

Where U and ρ are determined experimentally and M is the mean molecular weight in a binary liquid mixture

$$M = (X_1M_1 + X_2M_2) \qquad (3)$$

where M_1 and M_2 are molecular weights of constituent components.

Simple manipulation yields the following relation

$$U_{Nomoto} = [(X_1R_1+X_2R_2) / (X_1V_1+X_2V_2)]^3 \qquad (4)$$

The Van Dael and Vangeel Equation

Van Dael [12] obtained the relation for ultrasonic velocity in liquid mixtures as

$$1/(X_1M_1+X_2M_2)*1/U^2_{imx} = X_1/M_1U_1^2 + X_2/M_2U_2^2 \qquad (5)$$

where U_{imx} is the ideal mixing ultrasonic velocity in liquid mixture.U_1 and U_2 are ultrasonic velocities in species.

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The Impedance Relation

Impedance relation $U = \Sigma X_i Z_i \ / \Sigma X_i\rho_i$ (6)

where X_i mole fraction, $\rho_{t,}$ is the density of the mixture and Z_i is the acoustic impedance.

The Rao's Specific Velocity Method Relation

Rao's specific velocity method[14] $U = (\Sigma X_i r_i \rho)^3$ (7)

where X_i mole fraction, U_i is the ultrasonic velocity, ρ_t is the density of the mixture, r_i is the Rao's specific sound velocity = $Ui^{1/3}/\rho_i$ and Z_i is the acoustic impedance.

The Junjie Equation

Junjie equation $U_J = (X_1M_1/\rho_1+X_2M_2/\rho_2)/[\{X_1M_1+X_2M_2\}^{1/2}\{X_1M_1/\rho_1U_1^2+X_2M_2/\rho_2U_2^2)\}^{1/2}]$ (8)

where M_1, M_2 are molecular weights of constituent components.. ρ_1 and ρ_2 are the densities of constituent components.

Chi-Square Test for Goodness of Fit

According to Karl Pearson [25] Chi-square value is evaluated for the binary liquid mixtures under study using the Formula

$$\chi^2 = \sum_{i=1}^{N} (U_{mix(obs)} - U_{mix(cal)})^2 / U_{mix(cal)}) \quad (9)$$

where n is the number of data used.

Average Percentage Error (APE)

The Average percentage error [26] calculated using the relation

APE = 1/n Σ (Umix(obs) - Umix(cal)) / Umix(obs)) X100% (10)

where n is the number of data used.

$U_{mix(obs)}$ = experimental values of ultrasonic velocities

$U_{mix(cal)}$ = computed values of ultrasonic velocities

Molecular Association

The degree of intermolecular interaction or molecular association is given by

$\alpha = [U^2_{exp}/ U^2_{imx}] -1$

DISCUSSION

Tables 1(a), 2(a) and 3(a) show that the theoretical values of ultrasonic velocity computed by various theories, 1(b), 2(b) and 3(b) show deviations from experimental values along with interaction parameter. The limitations and approximations incorporated in these theories are responsible for it. It is assumed that all the molecules are spherical in shape, which is not true every time. In Nomoto's theory, it is supposed that the volume does not change on mixing. Therefore, no interaction between the components of liquid mixtures has been taken into account. The assumption for the formation of ideal mixing relation is that, the ratio of specific heats of ideal mixtures and the volumes are also equal. Again, no molecular interaction is taken into account. Similarly, as per the assumption for the Collision Factor theory, the molecules are treated as real non- elastic substances, which is not really the case. But on mixing two liquids, the interaction between the molecules of the two liquids takes place because of presence of various types of forces such as dispersion forces, charge transfer, hydrogen bonding, dipole - dipole and dipole – induced dipole interactions.

Thus, the observed deviation of theoretical values of velocity from the experimental values shows that the molecular interaction is taking place between the unlike molecules in the liquid mixture.

From tables 1(a) to 3(b), it is clear that for the binary systems of Ethyl benzoate and isomeric buatnol systems, there is a good agreement between experimental and theoretical values calculated by Impedance relations at all the temperatures. Theoretical values calculated by Nomoto's relation agree with the experimental values but not as near as from Impedance relations. The remaining theories show more deviations. The trends in the velocities in the studied mixtures can be explained on the basis of complex formation between ethyl benzoate and 2-alkanol molecules through hydrogen bonding between oxygen atom of ethyl benzoate and hydrogen atom of hydroxyl group in 2-alkanol molecules. .

There are higher variations in some intermediate concentration range suggesting the existence of strong tendency of association between component molecules as a result of dipole-dipole interactions. However, there is reasonably a good agreement between the experimental and theoretical velocities of Nomoto's relation and Impedance relation. Nomoto's theory proposes that the volume does not change upon mixing. Therefore, no interaction between the components of liquid mixtures has been taken into account. Similarly, the assumption for the formation of ideal mixing relation is that, the ratios of specific heats of ideal mixtures and the volumes are also equal. Again no

molecular interactions are taken into account. But upon mixing, interactions between the molecules occur because of the presence of various types of forces such as dispersion forces, charge transfer, hydrogen bonding dipole-dipole and dipole-induced dipole interactions. Thus, the observed deviation of theoretical values of velocity from the experimental values shows that the molecular interactions are taking place between the unlike molecules in the liquid mixtures. From the data it is observed that maximum positive deviation exhibiting a minimum of approximately 0.5 mole fraction for all the three systems at all the temperatures. The ratio U^2_{exp}/U^2_{imx} is an important tool to measure the non ideality in the mixtures especially in such cases where the properties other than sound velocity are not known.

Table 1(a)

Experimental and Theoretical Ultrasonic velocities (U m.sec^{-1}) of for the system Ethyl benzoate (EB) + 2-methyl-1-propanol

			303.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1112.0	1112.0	1112.0	1112.0	1112.0	1112.0
0.0670	1134.7	1141.1	1134.9	1084.4	1124.9	1192.4
0.1390	1158.5	1168.6	1157.9	1063.7	1140.4	1273.4
0.2168	1183.1	1194.8	1181.0	1049.9	1158.3	1352.1
0.3010	1208.7	1219.7	1204.3	1043.5	1178.5	1425.0
0.3924	1234.7	1243.3	1227.6	1045.4	1200.9	1488.3
0.4921	1261.0	1265.9	1251.1	1057.5	1225.5	1534.6
0.6011	1286.7	1287.4	1274.7	1083.2	1252.2	1556.2
0.7209	1310.9	1307.9	1298.4	1128.8	1281.1	1541.3
0.8532	1331.5	1327.5	1322.2	1206.6	1312.4	1476.4
1.0000	1346.2	1346.2	1346.2	1346.2	1346.2	1346.2
			308.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1104.0	1104.0	1104.0	1104.0	1104.0	1104.0
0.0670	1125.9	1132.3	1126.3	1076.5	1116.4	1186.7
0.1390	1148.8	1159.1	1148.8	1055.8	1131.4	1269.4
0.2168	1172.7	1184.5	1171.3	1042.0	1148.8	1349.1
0.3010	1197.3	1208.7	1193.9	1035.5	1168.4	1422.8
0.3924	1222.6	1231.7	1216.6	1037.2	1190.2	1486.2
0.4921	1248.0	1253.7	1239.5	1049.1	1214.1	1530.5
0.6011	1273.1	1274.6	1262.4	1074.3	1240.1	1549.8
0.7209	1296.7	1294.6	1285.5	1118.9	1268.4	1532.2
0.8532	1317.2	1313.7	1308.6	1195.3	1298.9	1467.2
1.0000	1331.9	1331.9	1331.9	1331.9	1331.9	1331.9
			313.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1096.5	1096.5	1096.5	1096.5	1096.5	1096.5
0.0670	1117.6	1123.7	1118.0	1069.0	1108.3	1180.4
0.1390	1139.6	1149.5	1139.7	1048.4	1122.6	1263.6
0.2168	1162.6	1174.1	1161.4	1034.5	1139.3	1344.4
0.3010	1186.3	1197.4	1183.2	1027.9	1158.2	1418.8
0.3924	1210.6	1219.5	1205.1	1029.3	1179.2	1481.7
0.4921	1235.1	1240.7	1227.1	1040.7	1202.3	1525.3
0.6011	1259.3	1260.8	1249.2	1065.2	1227.5	1545.1
0.7209	1282.0	1280.0	1271.4	1108.8	1254.7	1525.4
0.8532	1301.8	1298.4	1293.6	1183.2	1284.2	1456.7
1.0000	1316.0	1316.0	1316.0	1316.0	1316.0	1316.0
			318.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1089.6	1089.6	1089.6	1089.6	1089.6	1089.6
0.0670	1108.6	1115.6	1110.2	1062.1	1100.7	1175.3
0.1390	1129.9	1140.2	1130.8	1041.5	1114.3	1260.7
0.2168	1152.1	1163.6	1151.5	1027.5	1130.2	1342.3
0.3010	1175.0	1185.9	1172.4	1020.6	1148.3	1415.9
0.3924	1198.4	1207.0	1193.3	1021.7	1168.3	1478.4
0.4921	1222.0	1227.2	1214.2	1032.5	1190.4	1520.7
0.6011	1245.2	1246.4	1235.3	1056.2	1214.5	1535.4
0.7209	1267.0	1264.7	1256.4	1098.5	1240.5	1513.8
0.8532	1285.8	1282.2	1277.7	1170.7	1268.7	1443.7
1.0000	1299.0	1299.0	1299.0	1299.0	1299.0	1299.0

Table 1(b)

Percentage deviations from the theoretical velocities and interaction parameters (α) for the system Ethyl benzoate (EB) + 2-methyl-1-propanol

				303.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0670	0.5607	0.0176	-4.4373	-0.8641	5.0879	0.9996	0.0950
0.1390	0.8739	-0.0507	-8.1868	-1.5610	9.9152	1.0010	0.1863
0.2168	0.9882	-0.1741	-11.2601	-2.0927	14.2838	1.0035	0.2699
0.3010	0.9103	-0.3622	-13.6688	-2.4926	17.9027	1.0073	0.3417
0.3924	0.6987	-0.5718	-15.3345	-2.7366	20.5430	1.0115	0.3950
0.4921	0.3892	-0.7807	-16.1349	-2.8159	21.7012	1.0158	0.4218
0.6011	0.0512	-0.9320	-15.8128	-2.6834	20.9417	1.0189	0.4109
0.7209	-0.2274	-0.9483	-13.8900	-2.2670	17.5785	1.0192	0.3486
0.8532	-0.3031	-0.6948	-9.3789	-1.4323	10.8788	1.0140	0.2177
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				308.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0670	0.5647	0.0378	-4.3904	-0.8449	5.3976	0.9992	0.0939
0.1390	0.8933	-0.0041	-8.0928	-1.5161	10.5021	1.0001	0.1839
0.2168	1.0076	-0.1209	-11.1414	-2.0411	15.0390	1.0024	0.2665
0.3010	0.9533	-0.2828	-13.5119	-2.4149	18.8334	1.0057	0.3369
0.3924	0.7477	-0.4868	-15.1606	-2.6526	21.5626	1.0098	0.3893
0.4921	0.4551	-0.6821	-15.9407	-2.7177	22.6347	1.0138	0.4152
0.6011	0.1178	-0.8380	-15.6184	-2.5889	21.7368	1.0170	0.4044
0.7209	-0.1642	-0.8652	-13.7093	-2.1828	18.1603	1.0175	0.3430
0.8532	-0.2694	-0.6501	-9.2560	-1.3864	11.3850	1.0131	0.2144
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				313.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0670	0.5476	0.0389	-4.3456	-0.8339	5.6235	0.9992	0.0929
0.1390	0.8720	0.0053	-8.0032	-1.4886	10.8801	0.9999	0.1816
0.2168	0.9851	-0.1052	-11.0151	-2.0009	15.6382	1.0021	0.2629
0.3010	0.9322	-0.2625	-13.3562	-2.3657	19.5966	1.0053	0.3321
0.3924	0.7382	-0.4554	-14.9758	-2.5902	22.3953	1.0092	0.3833
0.4921	0.4506	-0.6492	-15.7414	-2.6539	23.4940	1.0131	0.4085
0.6011	0.1202	-0.8045	-15.4139	-2.5272	22.6962	1.0163	0.3977
0.7209	-0.1523	-0.8306	-13.5135	-2.1258	18.9876	1.0168	0.3369
0.8532	-0.2593	-0.6278	-9.1111	-1.3507	11.8957	1.0127	0.2105
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				318.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0670	0.6306	0.1414	-4.1901	-0.7135	6.0164	0.9972	0.0894
0.1390	0.9147	0.0811	-7.8272	-1.3799	11.5731	0.9984	0.1770
0.2168	1.0009	-0.0479	-10.8171	-1.8993	16.5086	1.0010	0.2573
0.3010	0.9248	-0.2246	-13.1430	-2.2755	20.5027	1.0045	0.3255
0.3924	0.7196	-0.4291	-14.7474	-2.5079	23.3609	1.0086	0.3759
0.4921	0.4235	-0.6352	-15.5065	-2.5844	24.4443	1.0128	0.4007
0.6011	0.0955	-0.7950	-15.1775	-2.4675	23.3040	1.0161	0.3899
0.7209	-0.1794	-0.8328	-13.3012	-2.0882	19.4780	1.0169	0.3304
0.8532	-0.2763	-0.6314	-8.9542	-1.3310	12.2769	1.0127	0.2064
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000

Figures 1-3 represents the variation of U^2_{exp}/U^2_{imx} with the mole fraction of Ethyl benzoate for isomeric buatnol binary systems studied, and the ratio of U^2_{exp}/U^2_{imx} gives an idea of extent of interaction taking place between molecules of the mixtures. The positive deviation for the systems infers strong interactions between the components. The percentage of deviation in velocity is reflecting both negative and positive magnitudes, indicating non ideal behaviour of liquid mixtures. The evaluated interaction parameters are positive for all the binary systems, indicating strong interactions between the mixing molecules [3]. The negative value of interaction parameter indicates the dominance of dispersion forces arising from the breakage of hydrogen bonds in the associates. But a positive value of (α) in all the system clearly indicates the existence of strong tendency for the formation of association in mixture through hydrogen bonding interactions and higher values of percentage deviation indicates maximum departure of the particular theory from experiment at that particular concentration and magnitude of the chi-square value finally determines the overall validity of the theory. The chi-square values along with average percentage error sigma are

given in the Table 4. From the values of chi-square and average percentage error it can be concluded that impedance relation is best suited.

Table 2(a)

Experimental and Theoretical Ultrasonic velocities (U m.sec^{-1}) of for the system Ethyl benzoate (EB) + 2-butanol

			303.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1152.0	1152.0	1152.0	1152.0	1152.0	1152.0
0.0750	1179.7	1172.8	1170.5	1137.7	1161.8	1232.3
0.1543	1206.6	1193.2	1189.3	1127.4	1173.6	1307.6
0.2382	1232.5	1213.4	1208.2	1121.5	1187.3	1374.3
0.3273	1257.2	1233.2	1227.3	1120.7	1203.0	1429.9
0.4219	1280.0	1252.7	1246.6	1125.9	1220.7	1471.3
0.5226	1300.6	1272.0	1266.1	1138.7	1240.7	1495.2
0.6300	1318.4	1291.0	1285.8	1161.3	1263.0	1497.2
0.7448	1332.5	1309.7	1305.7	1197.7	1287.9	1475.1
0.8678	1342.2	1328.1	1325.9	1254.8	1315.5	1425.3
1.0000	1346.2	1346.2	1346.2	1346.2	1346.2	1346.2
			308.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1142.5	1142.5	1142.5	1142.5	1142.5	1142.5
0.0750	1169.6	1162.7	1160.6	1128.2	1152.0	1223.3
0.1543	1196.1	1182.7	1178.9	1117.9	1163.3	1298.4
0.2382	1221.5	1202.3	1197.4	1112.0	1176.6	1365.0
0.3273	1245.5	1221.6	1216.0	1111.1	1191.9	1420.4
0.4219	1267.7	1240.7	1234.9	1116.1	1209.2	1461.6
0.5226	1287.7	1259.5	1253.9	1128.5	1228.7	1484.6
0.6300	1305.0	1278.0	1273.1	1150.7	1250.5	1486.1
0.7448	1318.7	1296.2	1292.5	1186.4	1274.8	1463.1
0.8678	1328.1	1314.2	1312.1	1242.4	1301.8	1412.2
1.0000	1331.9	1331.9	1331.9	1331.9	1331.9	1331.9
			313.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1137.5	1137.5	1137.5	1137.5	1137.5	1137.5
0.0750	1163.6	1156.6	1154.6	1123.0	1146.3	1218.2
0.1543	1189.1	1175.4	1171.8	1112.5	1156.9	1293.3
0.2382	1213.4	1193.9	1189.3	1106.3	1169.4	1359.6
0.3273	1236.4	1212.1	1206.8	1104.9	1183.8	1414.6
0.4219	1257.7	1230.1	1224.6	1109.4	1200.1	1454.6
0.5226	1276.7	1247.8	1242.5	1121.1	1218.5	1476.4
0.6300	1292.8	1265.2	1260.6	1142.3	1239.2	1476.6
0.7448	1305.4	1282.4	1278.9	1176.5	1262.1	1451.1
0.8678	1313.5	1299.3	1297.4	1230.3	1287.6	1398.4
1.0000	1316.0	1316.0	1316.0	1316.0	1316.0	1316.0
			318.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1132.8	1132.8	1132.8	1132.8	1132.8	1132.8
0.0750	1157.7	1150.6	1148.7	1118.1	1140.8	1213.5
0.1543	1181.9	1168.1	1164.8	1107.3	1150.6	1288.0
0.2382	1205.0	1185.4	1181.0	1100.7	1162.2	1353.6
0.3273	1226.8	1202.4	1197.4	1098.9	1175.6	1408.2
0.4219	1246.8	1219.1	1213.9	1102.7	1190.9	1447.1
0.5226	1264.5	1235.6	1230.6	1113.6	1208.1	1467.2
0.6300	1279.4	1251.8	1247.5	1133.6	1227.3	1465.6
0.7448	1290.8	1267.8	1264.5	1166.3	1248.8	1438.8
0.8678	1297.7	1283.5	1281.7	1217.5	1272.6	1383.7
1.0000	1299.0	1299.0	1299.0	1299.0	1299.0	1299.0

Table 2(b)

Percentage deviations from the theoretical velocities and interaction parameters (α) for the system Ethyl benzoate (EB) + 2-butanol

				303.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0750	-0.5882	-0.7764	-3.5639	-1.5148	4.4617	1.0157	0.0753
0.1543	-1.1096	-1.4363	-6.5669	-2.7365	8.3682	1.0294	0.1455
0.2382	-1.5532	-1.9725	-9.0058	-3.6691	11.5044	1.0406	0.2077
0.3273	-1.9089	-2.3782	-10.8574	-4.3135	13.7356	1.0493	0.2584
0.4219	-2.1289	-2.6087	-12.0375	-4.6295	14.9450	1.0543	0.2924
0.5226	-2.1986	-2.6514	-12.4513	-4.6050	14.9608	1.0552	0.3047
0.6300	-2.0803	-2.4707	-11.9173	-4.2007	13.5619	1.0513	0.2889
0.7448	-1.7141	-2.0082	-10.1162	-3.3496	10.7037	1.0414	0.2378
0.8678	-1.0530	-1.2171	-6.5091	-1.9898	6.1922	1.0248	0.1441
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				308.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0750	-0.5878	-0.7681	-3.5398	-1.5084	4.5879	1.0155	0.0747
0.1543	-1.1242	-1.4373	-6.5379	-2.7404	8.5565	1.0294	0.1448
0.2382	-1.5727	-1.9747	-8.9657	-3.6749	11.7519	1.0407	0.2067
0.3273	-1.9159	-2.3660	-10.7941	-4.3055	14.0461	1.0491	0.2566
0.4219	-2.1298	-2.5900	-11.9606	-4.6151	15.2926	1.0539	0.2902
0.5226	-2.1912	-2.6257	-12.3632	-4.5833	15.2902	1.0547	0.3020
0.6300	-2.0697	-2.4444	-11.8274	-4.1777	13.8799	1.0507	0.2863
0.7448	-1.7042	-1.9865	-10.0355	-3.3303	10.9481	1.0409	0.2355
0.8678	-1.0470	-1.2045	-6.4539	-1.9784	6.3291	1.0245	0.1427
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				313.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0750	-0.6027	-0.7742	-3.4880	-1.4888	4.6950	1.0157	0.0736
0.1543	-1.1532	-1.4512	-6.4438	-2.7078	8.7609	1.0297	0.1425
0.2382	-1.6066	-1.9893	-8.8305	-3.6271	12.0495	1.0410	0.2031
0.3273	-1.9617	-2.3903	-10.6339	-4.2563	14.4106	1.0496	0.2521
0.4219	-2.1935	-2.6317	-11.7908	-4.5776	15.6572	1.0548	0.2852
0.5226	-2.2629	-2.6767	-12.1866	-4.5552	15.6424	1.0558	0.2968
0.6300	-2.1315	-2.4886	-11.6438	-4.1498	14.2141	1.0517	0.2809
0.7448	-1.7606	-2.0297	-9.8722	-3.3157	11.1649	1.0419	0.2311
0.8678	-1.0785	-1.2287	-6.3336	-1.9683	6.4604	1.0250	0.1398
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				318.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0750	-0.6126	-0.7753	-3.4220	-1.4582	4.8222	1.0157	0.0721
0.1543	-1.1643	-1.4471	-6.3155	-2.6464	8.9770	1.0296	0.1394
0.2382	-1.6266	-1.9900	-8.6587	-3.5510	12.3325	1.0410	0.1986
0.3273	-1.9896	-2.3967	-10.4284	-4.1726	14.7824	1.0497	0.2464
0.4219	-2.2199	-2.6364	-11.5548	-4.4856	16.0684	1.0549	0.2784
0.5226	-2.2859	-2.6794	-11.9318	-4.4618	16.0335	1.0558	0.2893
0.6300	-2.1561	-2.4958	-11.3924	-4.0693	14.5535	1.0518	0.2737
0.7448	-1.7830	-2.0390	-9.6472	-3.2549	11.4633	1.0421	0.2249
0.8678	-1.0933	-1.2363	-6.1767	-1.9342	6.6306	1.0252	0.1360
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000

Table 3(a)

Experimental and Theoretical Ultrasonic velocities (U m.sec^{-1}) of for the system Ethyl benzoate (EB) + 2-methyl-2-propanol

			303.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1061.0	1061.0	1061.0	1061.0	1061.0	1061.0
0.0743	1087.8	1089.7	1088.7	1050.1	1073.6	1142.6
0.1529	1115.4	1118.4	1116.6	1043.3	1088.8	1221.1
0.2363	1143.7	1147.0	1144.6	1041.0	1106.8	1295.4
0.3250	1172.6	1175.6	1172.9	1043.9	1127.8	1361.7
0.4193	1202.0	1204.2	1201.3	1053.4	1152.3	1415.7
0.5199	1231.7	1232.7	1229.9	1071.4	1180.5	1454.2
0.6275	1261.4	1261.2	1258.7	1101.1	1213.1	1471.6
0.7428	1290.8	1289.6	1287.7	1147.8	1250.9	1462.7
0.8666	1319.3	1317.9	1316.8	1221.9	1294.8	1422.5
1.0000	1346.2	1346.2	1346.2	1346.2	1346.2	1346.2
			308.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1055.7	1055.7	1055.7	1055.7	1055.7	1055.7
0.0743	1081.5	1083.5	1082.6	1044.8	1067.8	1138.6
0.1529	1108.1	1111.2	1109.6	1037.8	1082.4	1218.3
0.2363	1135.3	1139.0	1136.8	1035.2	1099.8	1293.3
0.3250	1163.2	1166.7	1164.2	1038.0	1120.1	1360.0
0.4193	1191.6	1194.3	1191.7	1047.1	1143.8	1414.3
0.5199	1220.3	1222.0	1219.4	1064.6	1171.2	1451.9
0.6275	1249.1	1249.5	1247.3	1093.4	1202.8	1467.5
0.7428	1277.6	1277.0	1275.3	1139.0	1239.5	1456.2
0.8666	1305.5	1304.5	1303.5	1211.3	1282.1	1412.6
1.0000	1331.9	1331.9	1331.9	1331.9	1331.9	1331.9
			313.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1047.6	1047.6	1047.6	1047.6	1047.6	1047.6
0.0743	1072.6	1074.6	1073.8	1036.6	1059.2	1131.1
0.1529	1098.3	1101.5	1100.1	1029.6	1073.3	1211.9
0.2363	1124.7	1128.4	1126.6	1026.9	1090.1	1287.5
0.3250	1151.7	1155.3	1153.2	1029.4	1109.8	1354.6
0.4193	1179.2	1182.2	1180.0	1038.2	1132.8	1408.6
0.5199	1207.1	1209.1	1206.9	1055.3	1159.4	1445.2
0.6275	1235.2	1235.9	1233.9	1083.4	1190.2	1459.6
0.7428	1263.0	1262.6	1261.1	1127.9	1225.9	1446.4
0.8666	1290.1	1289.3	1288.5	1198.5	1267.4	1400.1
1.0000	1316.0	1316.0	1316.0	1316.0	1316.0	1316.0
			318.15K			
X_1	EXP	NOM	IMP	VDV	JUN	RAO
0.0000	1038.1	1038.1	1038.1	1038.1	1038.1	1038.1
0.0743	1062.3	1064.3	1063.6	1027.1	1049.3	1122.8
0.1529	1087.1	1090.5	1089.2	1020.0	1062.9	1203.9
0.2363	1112.7	1116.6	1115.0	1017.3	1079.2	1280.1
0.3250	1138.9	1142.8	1140.9	1019.6	1098.3	1347.4
0.4193	1165.6	1168.9	1166.9	1028.1	1120.6	1401.0
0.5199	1192.7	1195.0	1193.0	1044.7	1146.6	1437.1
0.6275	1220.0	1221.1	1219.3	1072.2	1176.5	1450.4
0.7428	1247.1	1247.1	1245.7	1115.7	1211.3	1435.1
0.8666	1273.6	1273.1	1272.3	1184.5	1251.7	1386.3
1.0000	1299.0	1299.0	1299.0	1299.0	1299.0	1299.0

Table 3(b)

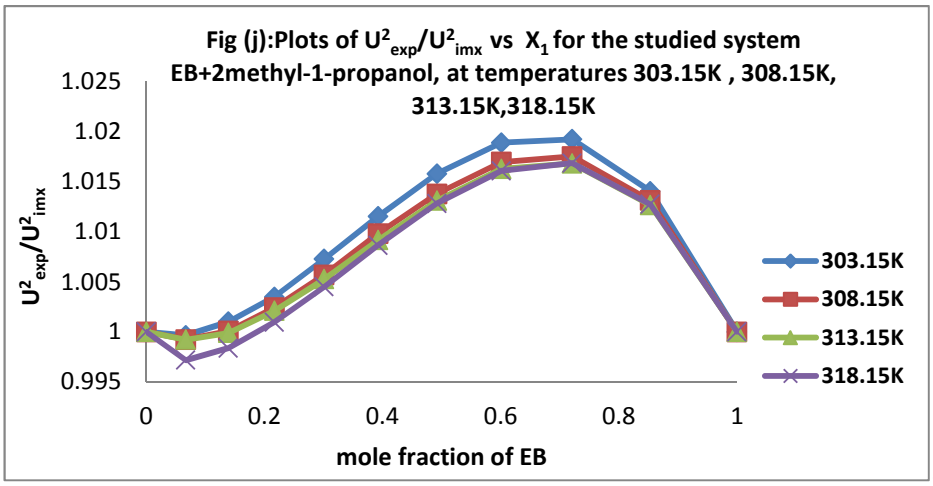
Percentage deviations from the theoretical velocities and interaction parameters (α) for the system Ethylbenzoate (EB) + 2-methyl-2-propanol

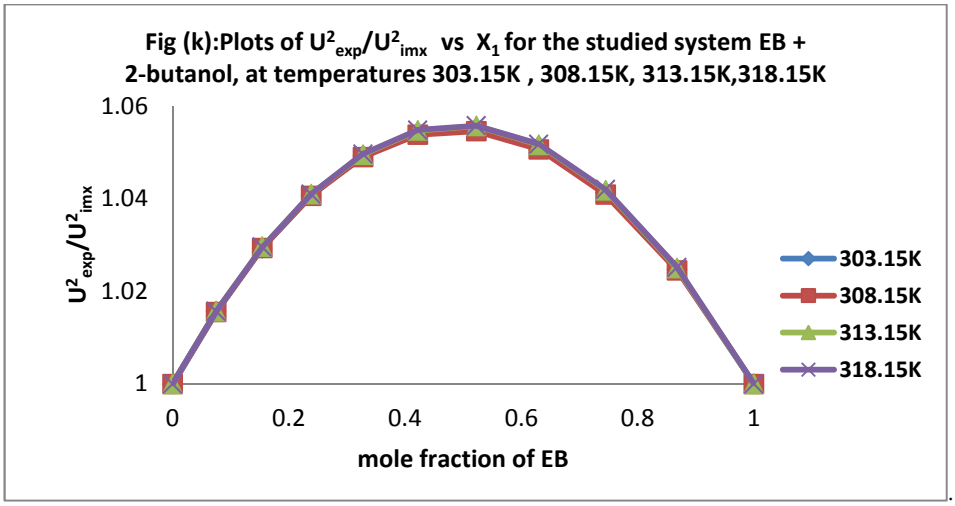
				303.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0743	0.1735	0.0820	-3.4616	-1.3044	5.0365	0.9984	0.0730
0.1529	0.2652	0.1043	-6.4645	-2.3830	9.4752	0.9979	0.1430
0.2363	0.2889	0.0800	-8.9832	-3.2252	13.2654	0.9984	0.2071
0.3250	0.2573	0.0213	-10.9728	-3.8166	16.1230	0.9996	0.2617
0.4193	0.1821	-0.0608	-12.3587	-4.1385	17.7767	1.0012	0.3019
0.5199	0.0822	-0.1481	-13.0115	-4.1585	18.0671	1.0030	0.3215
0.6275	-0.0172	-0.2165	-12.7116	-3.8293	16.6633	1.0043	0.3125
0.7428	-0.0937	-0.2437	-11.0808	-3.0940	13.3175	1.0049	0.2648
0.8666	-0.1037	-0.1872	-7.3790	-1.8587	7.8239	1.0038	0.1657
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				308.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0743	0.1821	0.0997	-3.3975	-1.2686	5.2760	0.9980	0.0716
0.1529	0.2819	0.1369	-6.3466	-2.3178	9.9436	0.9973	0.1401
0.2363	0.3221	0.1338	-8.8128	-3.1280	13.9162	0.9973	0.2026
0.3250	0.2975	0.0846	-10.7671	-3.7022	16.9209	0.9983	0.2559
0.4193	0.2290	0.0096	-12.1262	-4.0126	18.6882	0.9998	0.2950
0.5199	0.1355	-0.0728	-12.7614	-4.0270	18.9775	1.0015	0.3140
0.6275	0.0343	-0.1459	-12.4623	-3.7061	17.4860	1.0029	0.3050
0.7428	-0.0432	-0.1790	-10.8493	-2.9859	13.9797	1.0036	0.2582
0.8666	-0.0761	-0.1517	-7.2191	-1.7961	8.2060	1.0030	0.1617
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				313.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0743	0.1820	0.1106	-3.3534	-1.2512	5.4580	0.9978	0.0706
0.1529	0.2911	0.1652	-6.2574	-2.2779	10.3465	0.9967	0.1380
0.2363	0.3314	0.1677	-8.6942	-3.0784	14.4731	0.9967	0.1995
0.3250	0.3158	0.1305	-10.6177	-3.6378	17.6173	0.9974	0.2517
0.4193	0.2560	0.0648	-11.9532	-3.9373	19.4528	0.9987	0.2899
0.5199	0.1629	-0.0188	-12.5791	-3.9523	19.7252	1.0004	0.3085
0.6275	0.0545	-0.1029	-12.2866	-3.6431	18.1685	1.0021	0.2998
0.7428	-0.0289	-0.1476	-10.6931	-2.9376	14.5242	1.0030	0.2538
0.8666	-0.0585	-0.1247	-7.1002	-1.7585	8.5253	1.0025	0.1587
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
				318.15K			
X_1	% NOM	% IMP	% VDV	% JUN	% RAO	U^2_{EXP}/U^2_{IMP}	α
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
0.0743	0.1871	0.1220	-3.3105	-1.2283	5.6948	0.9976	0.0696
0.1529	0.3100	0.1952	-6.1701	-2.2274	10.7437	0.9961	0.1358
0.2363	0.3542	0.2047	-8.5780	-3.0137	15.0479	0.9959	0.1965
0.3250	0.3419	0.1725	-10.4786	-3.5631	18.3095	0.9966	0.2478
0.4193	0.2850	0.1102	-11.7971	-3.8564	20.1962	0.9978	0.2854
0.5199	0.1945	0.0282	-12.4126	-3.8693	20.4891	0.9994	0.3035
0.6275	0.0887	-0.0554	-12.1175	-3.5622	18.8813	1.0011	0.2948
0.7428	0.0002	-0.1086	-10.5404	-2.8709	15.0741	1.0022	0.2495
0.8666	-0.0411	-0.1017	-6.9933	-1.7183	8.8507	1.0020	0.1560
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000

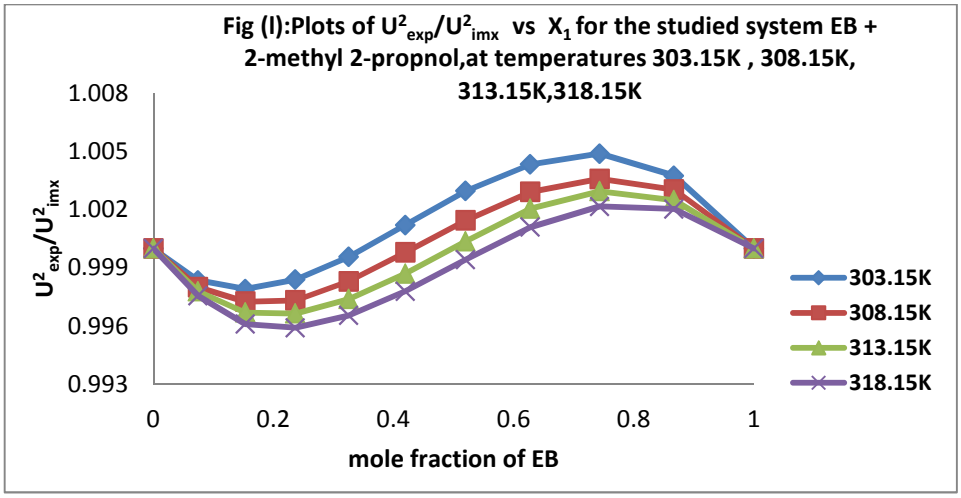
Table 4

Valus of chi-square and the relative deviation sigma for the binary mixtures of Ethylbenzoate (EB) at different temperatures

	χ^2					σ				
(EB + 2-methyl-1-propanol)										
T(K)	NOM	IMP	VDV	JUN	RAO	NOM	IMP	VDV	JUN	RAO
303.15	0.097	0.020	101.436	7.629	115.284	0.025	-0.010	-0.912	-0.233	0.790
308.15	0.201	0.005	104.228	7.853	114.871	0.037	0.003	-0.935	-0.239	0.795
313.15	0.324	0.031	106.620	8.108	114.469	0.047	0.014	-0.956	-0.245	0.801
318.15	0.451	0.081	109.478	8.473	113.819	0.057	0.024	-0.980	-0.253	0.806
(EB +2-butanol)										
T(K)	NOM	IMP	VDV	JUN	RAO	NOM	IMP	VDV	JUN	RAO
303.15	3.264	4.837	108.277	15.027	153.191	-0.146	-0.179	-0.925	-0.322	0.878
308.15	3.232	4.721	105.794	14.788	158.681	-0.146	-0.178	-0.918	-0.321	0.896
313.15	3.393	4.829	101.761	14.421	164.930	-0.150	-0.181	-0.902	-0.318	0.915
318.15	3.443	4.805	96.664	13.727	171.815	-0.152	-0.181	-0.881	-0.312	0.936
(EB +2-methyl-2-propanol)										
T(K)	NOM	IMP	VDV	JUN	RAO	NOM	IMP	VDV	JUN	RAO
303.15	0.036	0.024	111.939	11.446	207.564	0.010	-0.006	-0.967	-0.288	1.027
308.15	0.044	0.016	106.651	10.648	226.774	0.014	-0.001	-0.946	-0.279	1.072
313.15	0.049	0.016	102.532	10.170	242.639	0.015	0.002	-0.931	-0.274	1.108
318.15	0.057	0.018	98.591	9.627	258.791	0.017	0.006	-0.917	-0.268	1.146







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