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Comparison of Computational and Experimental Ultrasonic Velocities in Binary Mixtures at Different Temperatures

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Abstract : A Theoretical estimation of Ultrasonic velocity in the binary mixtures of Methyl Benzoate with 1-Propanol, 1-Butanol, 1-Pentanol has been carried out at different temperatures from 303-318K using Nomoto's relation, Impedance relation, Ideal mixture relation and Junjie's method. Theoretical values are compared with the experimental values and the validity of the theories is checked by applying the chi-square test for goodness of fit and by calculating the average percentage error (APE). It is found that the ultrasonic velocities evaluated using these theories are satisfactory to different extents in different mixtures.
Keywords: Theoretical Ultrasonic velocity, Binary mixtures, Methyl benzoate.

Introduction

Ultrasonic velocity plays a vital role in understanding the intermolecular interations in liquid mixtures between the polar and non polar component molecules. A variety of emperical, semiemperical and statistical formulas are available in the literature for the theoretical computation of ultrasonic velocity in liquids and their liquid mixtures[1-5]. Measurement of ultrasonic velocity gives the valuable information about the physicochemical behavior[6,7] of the liquid and liquid mixtures. In continuation of our dielectric work[8-10] we report the ultrasonic velocity evaluated using Nomoto's relation[1], Impedance relation[2], Ideal mixture relation[3], Junjie's method[4] for the binary mixtures of Methyl benzoate with 1-Propanol, 1-Butanol, 1-Pentanol at different temperatures from 303-318K. Further, the best suitable theory for the given molecular system under study is also picked out by calculating the average percentage error and chi-square test.

Experimental

Chemicals

The compounds Methyl benzoate, 1-Propanol, 1-Butanol, 1-Pentanol of 99% AR grade were supplied by Merck Co. Inc., Germany.

Measurements

The ultrasonic velocity was measured at different temperatures from 303-318K using a single crystal ultrasonic interferometer (M/s Mittal Enterprises, India) operating at a frequency of 2 MHz with an accuracy of 0.1m/s. The densities were also measured at different temperatures from 303-318K using specific gravity bottle method by the standard procedure. All the measurements were made using a constant temperature bath with in ±0.01K.

Results and Discussion

Ultrasonic velocities for the binary mixtures were determined at four different temperatures from 303-318K on the basis of different theories and relations as discussed earlier[11]. The validity of these theories was checked by applying Chi-square test and by calculating average percentage error. The values theoretical and experimental ultrasonic velocities are given in Table 1.

It can be seen from Table 1 that the theoretical values of ultrasonic velocity computed by various theories show deviation from experimental values. The predictive abilities of various ultrasonic theories depend upon the strength of interaction prevailing in a system. These theories generally fail to predict accurately the ultrasonic velocities where strong interactions are supposed to exist. The extent of deviation in the velocities may be attributed to the assumptions made in these theories for the non polar- polar and non polar-non polar interaction between the molecules.

The Chi-square value and APE value is minimum for Nomoto's relation than those obtained by other theories. An important reason for deviation from experimental values of ultrasonic velocity is that the molecular association effects are not taken into account in these theories. When two liquids are mixed, the interaction between the molecules of the two liquids takes place because of the presence of various forces like dispersive force, charge transfer, hydrogen bonding dipole-dipole and dipole-induced dipole interactions.

Hence the observed deviation shows that the molecular interaction is taking place between the unlike molecules in the liquid mixture[11]. Similar kinds of results were obtained by earlier workers[12,13,14,15]. The agreement between experimental and theoretical velocities of Nomoto's relation in all the three binary systems, suggests that R is additive property in all the systems. Higher deviations are observed in some intermediate concentration range. This suggests the existence of strong tendency for the association between component molecules as a result of Hydrogen bonding[16, 17].

The theories used at present are inadequate to explain the intermolecular interactions at the fullest, because in order to explain intermolecular interactions we at least need to know about the dipole dipole interactions, collision factors, hydrogen bond forces etc. Such an expression has not yet been developed.

Table 1. Experimental and computed values of *Ultrasonic velocity* at different temperatures.

Methyl benzoate + 1-Propanol										
X_1	303K					308K				
	U_{exp} ms^{-1}	U_{NOM} ms^{-1}	U_{IMR} ms^{-1}	U_{JM} ms^{-1}	U_{IMP} ms^{-1}	U_{exp} ms^{-1}	U_{NOM} ms^{-1}	U_{IMR} ms^{-1}	U_{JM} ms^{-1}	U_{IMP} ms^{-1}
0.0000	1195.2	1195.2	1195.2	1195.2	1195.2	1174.8	1174.8	1174.8	1174.8	1174.8
0.0604	1215.4	1215.4	1176.3	1211.7	1211.1	1195.8	1195.8	1148.6	1194.4	1190.2
0.1263	1236.8	1236.8	1160.6	1230.2	1227.7	1217.2	1217.2	1126.3	1214.0	1206.4
0.1986	1256.2	1256.2	1148.6	1248.1	1245.2	1236.8	1236.8	1108.3	1232.0	1223.4
0.2782	1277.0	1277.0	1141.1	1266.7	1263.7	1255.5	1255.5	1095.2	1251.8	1241.3
0.3664	1296.6	1296.6	1139.6	1285.8	1283.2	1273.8	1273.8	1088.2	1270.9	1260.1
0.4645	1317.0	1317.0	1146.0	1306.3	1303.8	1293.4	1293.4	1089.2	1289.3	1279.9
0.5743	1336.6	1336.6	1164.0	1327.7	1325.6	1312.2	1312.2	1101.4	1309.5	1300.9
0.6982	1358.0	1358.0	1200.1	1351.4	1348.7	1331.0	1331.0	1130.6	1330.4	1323.1
0.8388	1378.8	1378.8	1267.6	1375.3	1373.3	1351.4	1351.4	1188.9	1351.1	1346.6
1.0000	1399.4	1399.4	1399.4	1399.4	1399.4	1371.6	1371.6	1306.0	1371.6	1371.6
APE		0.0000	7.8445	0.4859	0.6310		0.0000	7.8523	0.1718	0.6817
Chi square		0.0000	135.86	0.4632	0.7683		0.0000	133.035	0.0659	0.8866
	313K					318K				
0.0000	1157.0	1157.0	1157.0	1157.0	1157.0	1142.4	1142.4	1142.4	1142.4	1142.4
0.0604	1178.7	1178.7	1131.0	1176.5	1172.1	1162.2	1162.2	1116.6	1161.0	1157.1
0.1263	1199.1	1199.1	1106.1	1195.3	1187.9	1184.1	1184.1	1094.6	1180.6	1172.5
0.1986	1219.7	1219.7	1098.1	1213.2	1204.6	1202.8	1202.8	1076.9	1197.5	1188.6
0.2782	1238.1	1238.1	1078.3	1232.1	1222.1	1220.7	1220.7	1064.1	1215.7	1205.4
0.3664	1255.7	1255.7	1071.4	1251.0	1240.5	1239.6	1239.6	1057.2	1233.6	1223.1
0.4645	1273.5	1273.5	1072.4	1269.2	1259.8	1256.7	1256.7	1058.1	1250.6	1241.7
0.5743	1292.3	1292.3	1085.5	1288.0	1280.3	1275.3	1275.3	1069.6	1269.2	1261.3

0.6982	1310.4	1310.4	1113.0	1308.1	1301.6	1291.9	1291.9	1097.5	1288.3	1281.9
0.8388	1330.2	1330.2	1170.0	1328.5	1324.4	1310.2	1310.2	1152.9	1307.5	1303.6
1.0000	1348.4	1348.4	1283.9	1348.4	1348.4	1326.6	1326.6	1263.2	1326.6	1326.6
APE		0.0000	7.9191	0.2608	0.7585		0.0000	7.8829	0.2891	0.7960
Chi square		0.0000	132.623	0.1333	1.0734		0.0000	130.392	0.1596	1.1725
Methyl benzoate + 1-Butanol										
X_1	303K					308K				
	$\mathbf{U_{exp}}$ **ms^{-1}**	U_{NOM} ms^{-1}	U_{IMR} ms^{-1}	U_{JM} ms^{-1}	U_{IMP} ms^{-1}	$\mathbf{U_{exp}}$ **ms^{-1}**	U_{NOM} ms^{-1}	U_{IMR} ms^{-1}	U_{JM} ms^{-1}	U_{IMP} ms^{-1}
0.0000	1217.4	1217.4	1217.4	1217.4	1217.4	1201.8	1201.8	1201.8	1201.8	1201.8
0.0738	1235.0	1235.0	1209.2	1242.8	1234.7	1218.4	1218.4	1193.5	1226.0	1218.0
0.1519	1252.0	1252.0	1203.9	1266.7	1252.2	1234.0	1234.0	1187.9	1248.0	1234.4
0.2350	1269.0	1269.0	1202.0	1288.6	1269.9	1249.2	1249.2	1185.7	1268.9	1250.9
0.3233	1286.8	1286.8	1204.2	1308.6	1287.9	1265.4	1265.4	1187.4	1287.1	1267.7
0.4175	1304.0	1304.0	1211.2	1326.2	1306.0	1282.2	1282.2	1193.7	1304.2	1284.7
0.5181	1321.4	1321.4	1224.3	1341.9	1324.4	1298.5	1298.5	1205.9	1318.9	1301.8
0.6258	1341.4	1341.4	1245.6	1358.1	1342.9	1316.7	1316.7	1226.0	1333.2	1319.0
0.7414	1360.8	1360.8	1277.8	1373.0	1361.6	1335.2	1335.2	1256.5	1347.1	1336.4
0.8658	1380.2	1380.2	1326.3	1386.9	1380.5	1352.4	1352.4	1302.4	1359.5	1354.0
1.0000	1399.4	1399.4	1399.4	1399.4	1399.4	1371.6	1371.6	1371.6	1371.6	1371.6
APE		0.0000	4.4758	0.2804	-0.065		0.0000	4.3219	-1.004	-0.104
Chi square		0.0000	41.6254	0.1453	0.014		0.0000	38.0620	1.9080	0.0269
	313K					318K				
0.0000	1190.6	1190.6	1190.6	1190.6	1190.6	1173.6	1173.6	1173.6	1173.6	1173.6
0.0738	1204.3	1204.3	1182.0	1213.9	1205.7	1188.8	1188.8	1165.1	1196.3	1188.3
0.1519	1220.3	1220.3	1176.2	1234.9	1221.0	1204.2	1204.2	1159.3	1217.2	1203.1
0.2350	1234.4	1234.4	1173.6	1254.1	1236.4	1217.3	1217.3	1156.6	1235.4	1218.1
0.3233	1248.0	1248	1174.8	1271.3	1252.0	1233.0	1233.0	1157.6	1252.7	1233.3
0.4175	1262.6	1262.6	1180.4	1287.3	1267.8	1247.0	1247.0	1163.1	1268.0	1248.6
0.5181	1279.6	1279.6	1191.8	1301.2	1283.7	1262.4	1262.4	1174.4	1281.7	1264.0
0.6258	1294.3	1294.3	1210.7	1313.9	1299.7	1276.8	1276.8	1192.5	1294.0	1279.5
0.7414	1312.3	1312.3	1239.5	1326.7	1315.8	1291.2	1291.2	1220.6	1306.1	1295.1
0.8658	1328.8	1328.8	1283.0	1337.4	1332.1	1309.2	1309.2	1262.9	1317.1	1310.8
1.0000	1348.4	1348.4	1384.4	1348.4	1348.4	1326.6	1326.6	1326.6	1326.6	1326.6
APE		0.0000	4.0972	-1.122	-0.210		0.0000	4.1969	-1.010	-0.078
Chi square		0.0000	33.6443	2.3184	0.0924		0.0000	34.7690	1.8442	0.0256
Methyl benzoate + 1-Pentanol										
X_1	303K					308K				
	$\mathbf{U_{exp}}$ **ms^{-1}**	U_{NOM} ms^{-1}	U_{IMR} ms^{-1}	U_{JM} ms^{-1}	U_{IMP} ms^{-1}	$\mathbf{U_{exp}}$ **ms^{-1}**	U_{NOM} ms^{-1}	U_{IMR} ms^{-1}	U_{JM} ms^{-1}	U_{IMP} ms^{-1}
0.0000	1248.4	1248.4	1248.4	1248.4	1248.4	1233.6	1233.6	1233.6	1233.6	1233.6
0.0871	1262.4	1262.4	1246.4	1279.6	1265.4	1245.1	1245.1	1231.2	1262.6	1249.1
0.1767	1276.2	1276.2	1246.9	1307.1	1281.9	1258.2	1258.2	1231.2	1289.0	1264.2
0.2690	1290.7	1290.7	1250.3	1327.8	1297.9	1270.8	1270.8	1233.9	1308.7	1278.9
0.3640	1305.2	1305.2	1256.7	1345.3	1313.6	1284.0	1284.0	1239.5	1325.1	1293.2
0.4619	1320.0	1320.0	1266.7	1359.4	1328.8	1297.0	1297.0	1248.5	1338.4	1307.1
0.5629	1334.6	1334.6	1280.8	1371.1	1343.6	1310.8	1310.8	1261.5	1349.2	1320.7
0.6670	1350.0	1350.0	1299.8	1378.9	1358.1	1325.6	1325.6	1279.1	1356.4	1333.9
0.7745	1366.4	1366.4	1324.8	1387.4	1372.2	1339.9	1339.9	1302.3	1363.8	1346.8
0.8854	1382.6	1382.6	1357.3	1394.6	1386.0	1355.6	1355.6	1332.5	1368.3	1359.3
1.0000	1399.4	1399.4	1399.4	1399.4	1399.4	1371.6	1371.6	1371.6	1371.6	1371.6
APE		0.0000	2.4603	3.1343	-0.407		0.0000	2.2870	-1.927	-0.464
Chi square		0.0000	12.2840	6.3318	0.3249		0.0000	10.4398	6.9599	0.4087
	313K					318K				
0.0000	1217.0	1217.0	1217.0	1223.8	1217.0	1201.4	1201.4	1201.4	1201.4	1201.4
0.0871	1228.6	1228.6	1214.4	1250.5	1231.8	1213.1	1213.1	1198.6	1227.6	1215.5

0.1767	1241.0	1241.0	1214.2	1275.4	1246.2	1224.6	1224.6	1198.2	1251.7	1229.2
0.2690	1253.7	1253.7	1216.6	1293.4	1260.2	1236.8	1236.8	1200.3	1270.8	1242.5
0.3640	1265.3	1265.3	1221.8	1309.2	1273.8	1249.8	1249.8	1205.2	1285.7	1255.5
0.4619	1276.8	1276.8	1230.4	1321.9	1287.0	1262.0	1262.0	1213.3	1299.8	1268.1
0.5629	1290.0	1290.0	1242.8	1331.8	1300.0	1274.3	1274.3	1225.2	1309.3	1280.4
0.6670	1303.8	1303.8	1259.6	1337.3	1312.5	1286.4	1286.4	1241.3	1316.2	1292.4
0.7745	1318.0	1318.0	1281.9	1343.3	1324.8	1300.2	1300.2	1262.7	1321.8	1304.1
0.8854	1332.8	1332.8	1310.8	1346.3	1336.7	1312.6	1312.6	1290.5	1324.8	1315.5
1.0000	1348.4	1348.4	1348.4	1348.1	1348.4	1326.6	1326.6	1326.6	1326.6	1326.6
APE		0.0000	2.2535	-2.182	-0.446		0.0000	2.3323	-1.789	-0.314
Chi square		0.0000	9.9205	8.3431	0.3815		0.0000	10.5721	5.8468	0.1800

Conclusion

It may be concluded that out of the four theories used at different temperatures, Nomoto's relation is best suited for all the binary mixtures under study. The Chi square values also support this theory. The observed deviation of theoretical values of velocity from the experimental values is attributed to the presence of intermolecular interactions and the extent of deviation is attributed

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