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PHYSICS

STRENGTH OF INTERACTION AND FORMATION OF HYDROGEN BONDING USING ULTRASONIC STUDIES

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Abstract

Using excess ultrasonic velocity in binary mixture, variation of velocity in one system has been found. Roa's and Vander Wall's constants have been calculated at maximum deviation to study the strength of interaction through hydrogen bonding. The results are analysed.

Keywords: Ultrasonics, Binary mixtures, Ultrasonic velocity, Ultrasonic density

Introduction

Ultrasonic velocity measurements in binary liquid mixtures and ternary mixtures have been employed to study the strength of interaction (1 – 3). Excess parameters in velocity, compressibility and volume have been computed to study interaction (4 – 5). In the present work, excess velocity, Roa's constant and Vander Wall's constant have been calculated for the following binary mixtures.

Theory and Calculations

Excess value of velocity in binary liquid mixtures can be found as

$$\Delta C = C_T - C_E$$

Where,
C_T - Velocity of mixtures in absent of interaction.

$C_T = C_1 X_1 + C_2 X_2$
Where,

X_1 & X_2 – Mole fractions of component 1 and 2.
C_1 & C_2 – Velocity of pure components
C_E – Experimental velocity of mixtures.

Changes in velocity by mixing second system can be obtain

$C_1^* = C_1 - \frac{\Delta C}{X_1}$

Knowing the value of C_1^*, the value of Vander Wall's constant 'b' and Rao's constant 'R' can be calculated for analyzing the hydrogen bonding (6,7).

$$b' = \frac{M}{\rho}\left[1 - \frac{RT}{MC_1^2}X_2\left\{\sqrt{\left(1 + \frac{MC_1^2}{2RT}\right)} - 1\right\}\right]$$

$$R' = \frac{M}{\rho}C_1^{2/3}$$

And percentage of increase over normal of b and R is obtained by

$\frac{b-b'}{b} \times 100$ and $\frac{R-R'}{R} \times 100$

b and R in pure state of component 1.

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Benzonitrile+Butan-1-ol

Table 1: Variation of ultrasonic velocity (C_1*) of binary liquid mixtures

Symbols and their meaning used in the following tables are φ_1- volume fraction of component 1, ρ – Density ($kg.m^{-3}$), C_{expt} – Experimental Velocity of mixtures ($m.s^{-1}$), C_{excess} – Excess value in velocity in binary mixtures ($m.s^{-1}$), C_1^* - Change in velocity by mixing the second system ($m.s^{-1}$), R – Rao's constant, b – Vander Wall's constant, R' – Rao's constant in pure state of component 1, b'- Vander Wall's constant in pure state of component 1.

φ_1	ρ	C exp	C excess	C_1^*
0.0369	810.4000	1235.9000	0.6831	1421.2119
0.1672	835.8000	1264.5000	6.6239	1442.3167
0.2355	849.4000	1278.2000	8.4466	1438.5665
0.3653	874.7000	1303.1000	10.7743	1432.1945
0.4372	888.5000	1314.2000	9.3709	1424.1339
0.5326	906.8000	1329.2000	7.7809	1417.3092
0.6484	928.7000	1347.1000	5.5432	1411.2491
0.8078	959.1000	1373.2000	3.9236	1407.5571
0.9667	989.1000	1399.9000	2.9909	1405.7939

Benzonitrile + Pentan-1-ol

0.0986	825.9000	1270.6000	0.1354	1404.0730
0.1552	836.8000	1279.1000	0.3322	1404.8402
0.2926	863.3000	1301.9000	2.9756	1412.8694
0.3745	878.8000	1315.9000	4.9609	1415.9466
0.4899	900.6000	1336.8000	8.9317	1420.9316
0.5959	920.3000	1354.5000	11.0815	1421.2962
0.7097	941.5000	1371.5000	11.3870	1418.7448
0.8120	960.4000	1383.2000	8.0796	1412.6502
0.9120	978.9000	1393.8000	4.0096	1407.0965

Benzonitrile + 2-Methylpropan-2-ol

0.0621	788.9000	1132.6000	4.4233	1473.9291
0.1649	811.8000	1177.6000	19.3338	1519.9454
0.3002	841.7000	1220.5000	22.6315	1478.0879
0.4190	867.8000	1256.5000	23.8587	1459.6420
	888.3000	1279.5000	19.5498	1440.8608

0.5123				
0.7444	938.4000	1339.3000	11.4141	1418.0333
0.8394	959.1000	1364.5000	8.8076	1413.1928
0.8997	972.5000	1376.9000	3.5578	1406.6544

Benzonitrile + Toluene

0.0974	871.8000	1304.9000	2.1178	1424.4435
0.1254	876.0000	1309.5000	3.6182	1431.5534
0.2138	888.9000	1321.2000	5.5323	1428.5762
0.3124	903.2000	1332.5000	5.9173	1421.6415
0.3844	913.5000	1340.8000	6.2469	1418.9511
0.4977	928.9000	1352.9000	5.8046	1414.3629
0.6304	946.7000	1364.9000	3.1147	1407.6409
0.7278	959.6000	1374.2000	1.6325	1404.9431
0.8496	975.5000	1386.8000	0.7493	1403.5819

1,1,1-Trichloroethane + 1-Propanol

0.2174	910.4200	1119.0000	- 17.3022	863.4131
0.3419	975.8300	1077.0000	-28.5507	859.4940
0.4499	1032.3300	1043.0000	-35.8747	863.2607
0.5454	1082.0600	1018.0000	-37.2862	874.6351
0.6293	1125.6400	998.0000	-36.5629	884.8991
0.6794	1156.7800	985.0000	-37.1882	888.2632
0.7327	1179.3600	977.0000	-32.0231	899.2944
0.8514	1241.2900	957.0000	-22.7042	916.3331
0.9317	1280.3400	949.0000	-10.8701	931.3330

1,1,1-Trichloroethane + 1-Butanol

0.0807	844.1200	1192.0000	-11.1619	804.6865
0.1947	903.5000	1149.0000	-21.8999	830.5198
0.2910	953.5100	1112.0000	-31.6470	834.2474
0.3846	1001.9900	1080.0000	-37.1582	846.3848
0.5004	1061.6300	1041.0000	-43.3868	856.2958
	1113.0600	1014.0000	-42.1434	872.7844

0.6002				
0.7038	1166.3600	987.0000	-39.8246	886.4149
0.7544	1192.5200	975.0000	-37.5048	893.2853
0.8383	1236.8600	960.0000	-28.7611	908.6912
0.9084	1272.6100	949.0000	-19.9228	921.0683

1,1,1-Trichloroethane + 1-Pentanol

0.1498	884.2900	1170.0000	-35.7118	704.6035
0.2047	912.3500	1147.0000	-41.7477	739.0542
0.3501	986.7100	1091.0000	-52.8191	792.1314
0.4621	998.8700	1079.0000	-30.2111	877.6222
0.5164	1071.2600	1039.0000	-53.4324	839.5290
0.6506	1139.8500	1004.0000	-46.9646	870.8134
0.7910	1211.9300	974.0000	-33.5810	900.5461
0.8955	1266.0000	954.0000	-21.2905	919.2250

1,1,1 – Trichloroethane + 1-Hexanol

0.0542	839.9100	1258.0000	-6.5720	821.7454
0.1388	882.9400	1217.0000	-18.8080	807.4957
0.2131	920.5800	1182.0000	-28.5460	809.0441
0.3176	973.4700	1137.0000	-38.0160	823.3023
0.4152	1022.8100	1197.0000	55.1680	1075.8709
0.5104	1071.0000	1063.0000	-46.4640	851.9655
0.6234	1128.2900	1027.0000	-44.0440	872.3487
0.6670	1150.4000	1014.0000	-42.2200	879.7016
0.7888	1212.5000	984.0000	-30.8080	903.9432
0.8983	1268.6300	962.0000	-15.5780	925.6584

1,1,1 – Trichloroethane + 1-Heptanol

0.1169	874.8600	1245.0000	-17.6822	791.7408
0.1515	892.2700	-23.1570	790.1485	1227.0000
0.2807	957.2500	1165.0000	-38.3866	806.2469
0.3896	1011.9400	1118.0000	-45.9648	825.0205
0.4387	1036.5500	1097.0000	-49.1906	830.8719

0.5768	1105.8500	1048.0000	-48.1984	859.4383
0.6603	1147.9100	1022.0000	-43.9714	876.4069
0.8464	1243.1900	975.0000	-23.6032	915.1134
0.9144	1276.9900	960.0000	-13.9872	927.7034

C_{exp} and ρ values taken from Ref: 9 and 10

Table 2: Percentage of increase in Vander wall's constant (b), Rao's constant (R)

Composition of Liquids	R	b	R'	b'	Percentage of increase in R	Percentage of increase in b
Benzonitrile + Butan-1-ol	1.0836	0.0966	1.0911	0.0967	-0.6960	-0.0786
Benzonitrile + Pentan-1-ol	1.1729	0.1046	1.1773	0.1047	-0.3798	-0.1463
Benzonitrile + 2-Methylpropan-2-ol	1.1206	0.0999	1.1306	0.1000	-0.8916	-0.1088
Benzonitrile + Tolune	1.1793	0.1051	1.1837	0.1052	-0.3775	-0.0791
1,1,1 Trichloroethane + 1-Propanol	0.9070	0.0975	0.9283	0.0976	3.1639	-0.1639
1,1,1 Trichloroethane + 1-Butanol	0.9587	0.1127	1.0662	0.1129	3.8001	-0.1649
1,1,1 Trichloroethane + 1-Pentanol	1.1083	0.1122	1.1535	0.1124	-4.4919	-0.0946
1,1,1 Trichloroethane + 1-Hexanol	1.1039	0.1122	1.1535	0.1124	-4.4919	-0.0946
1,1,1 Trichloroethane + 1-Heptanol	1.1707	0.1191	1.1224	0.1192	4.1319	-0.1390

Result and Discussion

The variation of velocity of one organic system (C1*) with addition of other organic system are mentioned in table (1). The percentage of increase of Vander walls constant(b) and Rao's constant(R) at maximum deviation is calculated and mentioned in table (2).

The deviation of velocity and compressibility from ideal mixture rule has been used to study the strength of interaction[9,10]. The values at maximum change of velocity in the composition, has been used calculate Vander wall's constant (b) and Rao's constant (R) to study CH-o and R CH-O bond strength. The values b and R in percentage are in expected range(b= -1.8%, R= -10.4% in water).

Percentage of increase of b is negative, this indicates CH-O bond in liquid mixture under study is less than water. Percentage of increase of R negative except 1,11,Ttrichloroethane composition. This may be attributed the fact that the R CH-O bond is less than water except the composition which is having chlorine atom. Even though this having polar property (this is attributed to the chlorine composition), the strength of interaction through R CH - O is less than water.

Conclusion

From the work the molecular interaction in the mixture is studied from values of percentage of increase in R and b.

The variation of velocity C_1^* indicates the individuality of the first component is changing with addition of second component.

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