Estimation of acoustic impedance, its excess value and molar sound velocity of the binary mixture of 2-Butanol and m-Xylene for different compositions at different temperatures

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ABSTRACT

Measurements of physico-acoustic properties at an ultrasonic level have been studied intensively for the binary mixture of 2-Butanol + m-Xylene system as a function of the composition at 298.15K to 323.15K by 5K intervals and at atmospheric pressure. Acoustic impedance (Z), excess acoustic impedance (Z^E) and molar sound velocity (R) have been evaluated from the experimental values of speeds of sound and densities. The variation of these properties with composition and temperature suggests the presence of dipole-induced dipole interactions, hydrogen bond, induced electrostatic and dispersion forces. The observed negative values of Z^E over the entire composition range of the system reinforce significant interactions between unlike molecules that dominate over other types. The variation of molar sound velocity (R) of the entire mixture suggests the rarefaction of the liquid mixture under study.

1. INTRODUCTION

From the very earlier time, the scientists and the physical chemists show greater interest in the term of mixture properties. A mixture is nothing but the interaction of different molecules. So the appearance of some new phenomena different from their individual pure states may be observed. By studying the liquid-liquid mixture at different mole fractions, the trend of changing of properties can find out. The temperature also does a strong effect on this change when liquids are mixed together; therefore, there may be either contraction or expansion in volume and thus deviating from the additive rule [1,2,3,4]. Still, today liquids have been studied extensively by both theoretical and experimental techniques using various physicochemical properties. Knowledge of ultrasonic velocity and density of different mole fractions of solvent-solute mixtures can further be used to determine the acoustic impedance, excess acoustic impedance and molar sound velocity. Sound generally travels through materials under the influence of sound pressure. As molecules or atoms of a compound are bound elastically to each other, the excess pressure results in a wave propagating through the compound. Among the sound properties, acoustic impedance is important i. in determining the acoustic transmission and reflection at the boundary of two materials having different acoustic impedances, ii. In designing ultrasonic transducers and iii. In assessing absorption of sound in a medium. Molar sound velocity, on the other hand, provides a clear idea on the intermolecular interactions occurred in any liquid mixture.

Alcohols, in particular, 2-Butanol (or 2-Bu-OH) is an organic compound normally found as an equal mixture of the two stereoisomers [5], a racemic mixture of (R)-(−)-2-Bu-OH and (S)-(+)-2-Bu-OH. This secondary alcohol is a flammable, colourless liquid that is soluble in water and completely miscible with polar solvents such as ethers and other alcohols [6,7], m-Xylene (or m-Xln) is an aromatic hydrocarbon, based on benzene with two methyl substituents. Generally, xylene is used as solvent & is most widely used as a clearing agent [8,9]. m-Xln is a common component of ink, rubber, and adhesive and In thinning paints and varnishes [10,11]. In the petroleum industry, m-

Xln is also a frequent component of paraffin solvents. It is also used as a raw material in the manufacture of 2,4- and 2,6-xylidine as well as a range of smaller-volume chemicals.

One most important application of these two liquids is both of them are frequently used in the pharmaceutical sector as residual solvents in the formulation of various essential drugs. So it is urgent to evaluate the mixing properties of this binary mixture to estimate the nature of mixing. The systematic survey of the literature shows that there is no systematic study especially on acoustic properties (acoustic impedance, molar sound velocity) present in the binary mixture containing 2-Bu-OH and m-Xln for every specific proportion along with the temperature. In view of this importance, it is of interest to study the physico-acoustic properties to estimate their acoustic nature in the mixture along with identifying the trend of changing for different molecular composition very intensively to understand the molecular interactions between them.

2. EXPERIMENTAL

The chemical reagents employed were of analytical graded and were obtained from Sigma Aldrich, England, with a minimum purity of 99.5%. The water used in all experimental works was double distilled. The binary mixtures of 2- Bu-OH and m-Xln were prepared by using an analytical balance with a precision of ± 0.1 μg and later were converted to the different components of the mixture using the dilution method. Special care was taken to prevent evaporation and the introduction of moisture into the experimental samples.

The density and speed of sound of all binary mixtures, including pure solvents, were measured using an oscillatory densimeter (Anton Paar DSA 5000). The temperature was automatically controlled with an uncertainty of ± 0.01K. The apparatus was calibrated frequently by measuring the double-distilled water and dry air. The uncertainty of density for all the solvent systems studied is less than ± 0.00005 gcm^{-3}, and the uncertainty of speed of sound is less than ± 1 ms^{-1}.

3. RESULTS AND DISCCUSION

The density values of binary mixtures, including m-Xln as a function of the mole fraction of 2-Bu-OH(x1) at temperatures (298.15 to 323.15) K are listed in Table 1. It is found that the density decreases as the temperature increases as well as with the increasing proportion of 2-Bu-OH. Corresponding speeds of sound are shown in Table 2. Here the existence of weak electrostatic force between the interacting molecules changes their structures. The structural changes affect the compressibility, and hence there is a sharp change in ultrasonic velocity. It is noticed regarding u at all temperatures in the order: m-Xln > 2-Bu-OH and with the addition of 2-Bu-OH, u decreases slowly for 2-Bu-OH + m-Xln system (Table 2).

TABEL I. Density of 2-Bu-OH + m-Xln system for different molar ratios at 298.15 K to 323.15 K by 5 K intervals

Mole fraction of X		**Experimental Density (ρ) ×10^{-3} (kg m^{-3})**					
2-Bu-OH x_1	**m-Xln x_2**	**298.15 K**	**303.15 K**	**308.15 K**	**313.15 K**	**318.15 K**	**323.15 K**
0.0000	1.0000	0.8599	0.8555	0.8512	0.8469	0.8425	0.8381
0.0500	0.9500	0.8569	0.8525	0.8481	0.8437	0.8392	0.8348
0.1007	0.8994	0.8542	0.8497	0.8453	0.8408	0.8363	0.8318
0.1499	0.8501	0.8516	0.8471	0.8426	0.8381	0.8336	0.8290
0.1998	0.8002	0.8486	0.8442	0.8396	0.8351	0.8305	0.8259

0.2496	0.7504	0.8460	0.8415	0.8369	0.8324	0.8278	0.8231
0.2998	0.7002	0.8433	0.8388	0.8343	0.8297	0.8251	0.8204
0.3498	0.6502	0.8407	0.8362	0.8316	0.8270	0.8223	0.8177
0.3996	0.6004	0.8381	0.8335	0.8290	0.8243	0.8197	0.8150
0.4498	0.5502	0.8354	0.8309	0.8263	0.8217	0.8170	0.8123
0.4993	0.5008	0.8328	0.8282	0.8236	0.8190	0.8143	0.8096
0.5490	0.4510	0.8300	0.8254	0.8209	0.8162	0.8115	0.8068
0.5997	0.4003	0.8272	0.8226	0.8180	0.8134	0.8087	0.8040
0.6493	0.3507	0.8246	0.8201	0.8155	0.8109	0.8062	0.8014
0.7026	0.2974	0.8213	0.8168	0.8123	0.8076	0.8029	0.7982
0.7497	0.2503	0.8185	0.8140	0.8095	0.8048	0.8002	0.7954
0.8001	0.1999	0.8156	0.8112	0.8067	0.8021	0.7974	0.7927
0.8483	0.1518	0.8128	0.8084	0.8039	0.7994	0.7947	0.7900
0.9009	0.0991	0.8092	0.8049	0.8004	0.7959	0.7913	0.7866
0.9503	0.0497	0.8059	0.8016	0.7973	0.7928	0.7882	0.7836
1.0000	0.0000	0.8027	0.7985	0.7942	0.7898	0.7853	0.7807

TABEL II. Sound Velocity of 2-Bu-OH + m-Xln system for different molar ratios at 298.15 K to 323.15 K

Mole fraction of X		**Speed of sound (u)** (m/s)					
2-Bu-OH x_1	**m-Xln x_2**	**298.15 K**	**303.15 K**	**308.15 K**	**313.15 K**	**318.15 K**	**323.15 K**
0.0000	1.0000	1317.99	1297.32	1276.82	1256.52	1236.44	1216.99
0.0500	0.9500	1308.42	1288.19	1268.11	1248.16	1228.37	1209.08
0.1007	0.8994	1299.39	1279.25	1259.31	1239.53	1219.92	1200.89
0.1499	0.8501	1292.12	1272.15	1252.15	1232.44	1212.90	1193.94
0.1998	0.8002	1285.32	1265.32	1245.51	1225.85	1206.37	1187.45
0.2496	0.7504	1279.04	1259.12	1239.37	1219.77	1200.34	1181.48
0.2998	0.7002	1273.24	1253.37	1233.67	1214.12	1194.74	1175.93
0.3498	0.6502	1267.81	1248.00	1228.33	1208.84	1189.50	1170.71
0.3996	0.6004	1262.79	1243.04	1223.75	1203.89	1184.57	1165.80

0.4498	0.5502	1258.00	1238.25	1218.66	1199.21	1179.91	1161.17
0.4993	0.5008	1253.42	1233.68	1214.12	1194.68	1175.40	1156.65
0.5490	0.4510	1248.84	1229.14	1209.61	1190.20	1170.92	1152.19
0.5997	0.4003	1244.46	1224.84	1205.34	1185.95	1166.70	1147.93
0.6493	0.3507	1240.90	1221.35	1201.90	1182.56	1163.32	1144.62
0.7026	0.2974	1236.32	1216.86	1197.48	1178.17	1158.96	1140.24
0.7497	0.2503	1232.60	1213.26	1193.88	1174.62	1155.43	1136.74
0.8001	0.1999	1228.92	1209.69	1190.53	1171.39	1152.30	1133.68
0.8483	0.1518	1225.11	1206.13	1187.16	1168.20	1149.33	1130.75
0.9009	0.0991	1220.34	1201.56	1182.76	1163.93	1145.09	1126.65
0.9503	0.0497	1215.98	1197.49	1178.97	1160.38	1141.73	1123.46
1.0000	0.0000	1211.83	1193.70	1175.57	1157.15	1138.84	1120.79

The acoustic impedance of a material is the displacement of the medium's particles by sound energy. It is one of the basic parameters to understand the intrinsic and elastic properties of the medium. Acoustic impedance (Z) and excess values of acoustic impedance (Z^E) are estimated by using Eq. (1,2) [12,13,].

$$Z = \rho u \tag{1}$$

$$Z^E = Z - (X_1 Z_1 + X_2 Z_2) \tag{2}$$

Experimentally obtained values of excess properties (Z^E) for this system can be fitted by a least square method using Redlich-Kister Eq. (3) [14]:

$$(Y)^E = x_1 x_2 \sum_{i \geq 0} (1 - 2x_1) B_i \tag{3}$$

$$R = VU^{1/3} \tag{4}$$

Where, x_1, x_2 is the mole fraction of component 1 and 2 and Bi the coefficient of Redlich-Kister equation. Another very important parameter is molar sound velocity which was calculated following Eq. (4) [15]. The estimated values of Z in the full range of composition $0 \leq x1 \leq 1$ between 298.15 K and 323.15 K are graphically represented by Figure 1. As acoustic impedance is one of the critical parameters that can be used to understand the intrinsic and elastic properties of the medium so this decreasing of Z values with the increasing proportion of 2-Bu-OH suggests that the existence of significant molecular interaction gradually increases. The estimated values of Z^E in the full range of composition of the system are represented in Figure 2.

By examining Figure (1,2) the following observations are noticed regarding Z and Z^E

1. At all temperatures, Z of the pure liquids varies in the order: *m-Xln > 2-Bu-OH.*
2. With the addition of 2-Bu-OH, Z decreases almost linearly to reach the value of pure alcohol.

3. Z^E values are negative over the whole range of composition within the studied range of temperatures.
4. As the alcohol concentration raises the negative Z^E values for both systems increases sharply until they reach the pick of the curve, after which decrease slowly toward pure alcohol.
5. The negative maxima of Z^E for 2-Bu-OH + m-Xln system found at $x_1 \approx 0.35$.

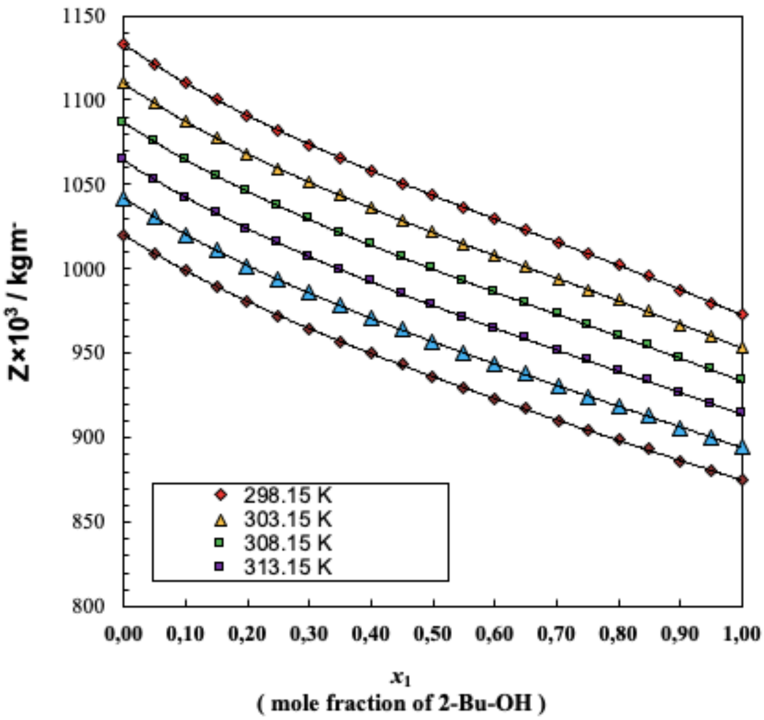

Figure 1. Acoustic impedance curve for different mole fractions at different temperatures. The graph presents the linear decreasing trend that indicates the significant interactions between the mixture components in a much-disciplined way.

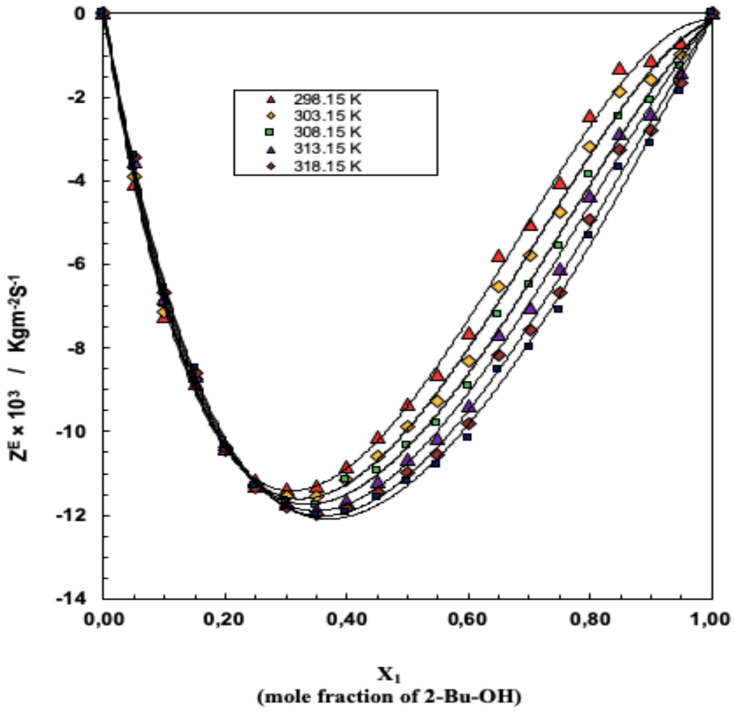

Figure 2. Excess acoustic impedance curve for different mole fractions at different temperatures. Negative excess values indicate the compactness due to molecular rearrangement and the extent of molecular interactions in liquid mixtures.

Here Z of m-Xln > 2-Bu-OH and thus there is almost a linear decrease of Z for the binary mixture with the increasing mole fraction of 2-Bu-OH. Negative excess values play a vital role in assessing the compactness due to molecular rearrangement and the extent of molecular interactions in liquid mixtures. The specific attraction between these unlike molecules is for physical intermolecular forces including electrostatic and induction forces between a permanent dipole and an induced dipole. Thus structural characteristics of the component arise from the regular fitting of one component into other structure due to the differences in shape and size of the components. They were breaking hydrogen bonds of adjacent alcohol molecules also responsible for negative excess values which also indicate strong molecular interaction between the, unlike molecules.

TABLE III. Molar sound velocity of 2-Bu-OH + m-Xln system for different molar ratios at different temperatures

Mole fraction of X		Molar sound velocity (Rao's Constant R) of 2-Bu-OH + m-Xln system for different molar ratios at different temperatures $(m^3/mol)(m/s)^{1/3}$					
2-Bu-OH x_1	m-Xln x_2	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0.0000	1.0000	1353.6370	1353.3280	1353.0190	1352.7150	1352.4330	1352.3070
0.0500	0.9500	1334.5770	1334.5080	1334.4340	1334.3570	1334.2790	1334.3110

0.1007	0.8994	1315.0390	1315.0510	1315.0870	1315.1410	1315.2170	1315.4400
0.1499	0.8501	1296.3450	1296.4380	1296.4970	1296.6160	1296.7630	1297.0700
0.1998	0.8002	1278.0930	1278.1940	1278.3340	1278.5010	1278.7100	1279.0850
0.2496	0.7504	1259.5400	1259.6760	1259.8530	1260.0600	1260.3120	1260.7340
0.2998	0.7002	1240.9260	1241.0820	1241.2830	1241.5190	1241.8050	1242.2650
0.3498	0.6502	1222.4340	1222.6150	1222.8310	1223.0970	1223.4090	1223.8950
0.3996	0.6004	1204.0830	1204.2780	1204.6130	1204.7770	1205.1070	1205.6080
0.4498	0.5502	1185.5840	1185.7880	1186.0370	1186.3320	1186.6790	1187.2090
0.4993	0.5008	1167.3850	1167.5880	1167.8480	1168.1510	1168.5130	1169.0470
0.5490	0.4510	1149.1860	1149.3960	1149.6630	1149.9770	1150.3430	1150.8900
0.5997	0.4003	1130.6220	1130.8440	1131.1150	1131.4310	1131.8080	1132.3460
0.6493	0.3507	1112.3450	1112.5700	1112.8420	1113.1660	1113.5460	1114.1060
0.7026	0.2974	1093.0670	1093.2940	1093.5710	1093.8930	1094.2730	1094.8270
0.7497	0.2503	1075.9850	1076.2140	1076.4740	1076.7960	1077.1750	1077.7310
0.8001	0.1999	1057.4670	1057.6900	1057.9690	1058.2910	1058.6700	1059.2270
0.8483	0.1518	1039.7570	1039.9920	1040.2750	1040.6040	1041.0100	1041.5430
0.9009	0.0991	1020.7530	1020.9770	1021.2500	1021.5650	1021.9380	1022.4790
0.9503	0.0497	1002.7090	1002.9310	1003.2020	1003.5190	1003.8880	1004.4240
1.0000	0.0000	984.4760	984.7010	984.9890	985.2700	985.6580	986.1860

Molar sound velocity or Rao's constant (R) gives a clear idea about the extent of interactions taking place between the molecules of this system. It indicates whether there are associative or dissociative interaction occurs. The variation of molar sound velocity listed in Table 3 shows that R is not constant for different molar ratios, so the interactions of this mixture are expected to be associative. However, the decreasing trend of the molar sound velocity with the increasing mole fraction of 2-Bu-OH suggests that the rarefaction of the medium.

4. CONCLUSIONS

The purpose of this work is to evaluate the acoustical impedance and molar sound velocity of this binary mixture and thus to determine how sound energy correlates through molecular levels of this mixture and how the intermolecular interactions of it change. Acoustic impedance is an essential characteristic of materials for nearly all sonic and ultrasonic applications. In the electrical analogy, it determines the efficiency of every transmission in the system from one element to another. In this study, the experimental densities and speed of sound of 2-Bu-OH, m-Xln and their binary system have been measured at temperatures (298.15 to 323.15) K and in atmospheric pressure. Excess acoustical impedance (Z^E) of this binary mixture was calculated and fitted with the Redlich–Kister equation. From these parameters, we got clear ideas about valuable acoustic properties as well as about the existing interactions between these mixing components, which are mainly for dipole–induced dipole interaction, induced electrostatic and dispersion force. The observed negative excess values ZE indicate the significant interaction between the different molecules, whereas R values suggest that the overall mixing is associative.

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