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Experimental and theoretical evaluations-excess ultrasonic speeds in binary liquid mixture at different temperatures

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ABSTRACT

The Ultrasonic speeds (U) of binary liquid mixture of 1,4-dioxane with 1-pentanol including those of pure liquids, over the entire composition range expressed by mole fraction x_1 of 1,4 dioxane was measured at temperatures (298.15, 303.15, 308.15, 313.15, and 318.15) K. From the experimental data, calculated the various theoretical evaluations viz., Nomoto, Impedance, Van dael and Vangeel, Rao's specific velocity and Junjie's for the binary mixture. Theoretical values are compared with the experimental values and molecular interaction parameter (α) is evaluated for understanding the different kinds of association, molecular packing and various types of intermolecular interactions. Using experimental ultrasonic speeds, excess ultrasonic speeds (U^E) are reported. A good agreement has been found between experimental and theoretical values of ultrasonic speeds. The relative applicability of these theories to the present system has been checked and discussed. The results are explained in terms of molecular interactions occurring in the binary liquid mixture and the negative excess ultrasonic speeds conforms existence of strong specific interactions in the mixture.

Keywords: Ultrasonic speeds, 1,4-dioxane, 1-pentanol, molecular interactions, Theoretical models.

INTRODUCTION

An excellent theoretical study explains all the known facts, which in turn can be verified by experimental while there are many techniques available to study the physical properties for interpreting the molecular interaction in liquids and liquid mixtures. The study for ultrasonic wave through the solution is found to be quite interesting. The ultrasonic wave through the solution is used for knowing the nature and strength of intermolecular interactions in pure liquids and the mixtures. There are two methods for evaluation of physical properties of mixtures. They are experimental and theoretical. Out of these the theoretical evaluation of sound velocity in liquid mixtures created a considerable interest among the researchers. Sound speed measurement gives the valuable information about physicochemical behavior of binary liquid mixtures [1-5]. Several researchers [6-9] carried out ultrasonic investigations on liquid mixtures and correlated the experimental results of ultrasonic speeds with theoretical relations of ultrasonic speeds in these mixtures were theoretically calculated by using Nomoto, impedance relation, Van dael and Vangeel, Rao's specific velocity, and Junjie's relations for the binary mixture and are compared with the experimental values over the entire range of composition at five different temperatures (298.15, 303.15, 308.15, 313.15 and 318.15) K. The suitability of these theories and relations was checked by comparing theoretical values of ultrasonic speeds with the values obtained experimentally. Using the values of experimental and theoretical ultrasonic speeds one can compute molar interaction parameter (α). The variations of this parameter with composition of mixture indicate the existence of molecular interactions in the mixture. Further, the excess ultrasonic speeds coefficients and there standard deviations are calculated using Redlich-Kister polynomial equation.

MATERIALS AND METHODS

The binary liquid mixture of 1, 4 dioxane and 1-pentanol with mass fraction purities >0.998 were purchased from Sigma Aldrich Chemical Co. the chemicals were prepared in airtight stopped glass bottles. Mole fractions of these samples were determined by measuring the mass of each component with a precision balance (Sartorius, model CP 225D, (0.01mg). The uncertainty of the composition on a mole fraction basis was 0.0001. The ultrasonic speeds of pure components and binary mixtures at different temperatures were obtained with a vibrating-tube densimeter (Anton Paar DMA 5000 M). The densimeter was calibrated with ultra pure water, and the ultrasonic speeds have been listed in Table 1, compared with literature.

Table -1: Observed and literature values of ultrasonic speeds, for the binary liquid mixture

Compound	T/K	Ultrasonic speeds (U)	
		Observed	Literature
	298.15	1344.3	1344.8 [10,11]
1,4-dioxane	303.15	1322.3	
	308.15	1300.5	1325 [12,13]
	298.15	1275.8	1275.2 [14]
1-Pentanol	303.15	1258.9	1263 [15,16]
	308.15	1242.2	

THEORY

The different theoretical considerations for the empirical formula for sound speed in binary liquid mixtures given by

Nomoto's: $U_N = \left[\dfrac{x_1R_1 + x_2R_2}{x_1V_1 + x_2V_2}\right]^3$

Impedance dependence: $U_{IMP} = \dfrac{\sum x_i Z_i}{\sum x_i \rho_i}$

Van Dael and Vangeel Ideal Mixture : $U_{VAN} = \left[\left(\dfrac{x_1}{M_1U_1^2} + \dfrac{x_2}{M_2U_2^2}\right)\right]^{-1/2}\left[\dfrac{1}{(x_1M_1 + x_2M_2)}\right]^{1/2}$

Rao's specific sound velocity: $U_R = \left(\sum x_i r_i \rho_i\right)^3$

Jungie's: $U_{JR} = \left[\dfrac{(x_1V_1 + x_xV_2)}{(x_1M_1 + x_2M_2)^{1/2}}\right] * \left[\dfrac{x_1V_1}{\rho_1U_1^2} + \dfrac{x_2V_2}{\rho_2U_2^2}\right]^{-1/2}$

Molecular interaction parameter: $\alpha = \left[\left(\dfrac{U_{Exp}}{U_{Theo}}\right)^2 - 1\right]$

where x_1, x_2 are mole fractions, M_1, M_2 are molecular weights, R is the molar sound speed, Z_i is acoustic impedance, ρ_i density of the i^{th} component of constituent components, of 1, 4-dioxane and 1-pentanol respectively, at the temperature range. (298.15, 303.15, 308.15, 313.15, and 318.15) K.
For Excess ultrasonic speeds calculated using the formula

$$Y^E = Y_{mix} - (x_1y_1 + x_2y_2) \tag{1}$$

where x_1 and x_2 are mole fractions of 1,4-Dioxane and 1-Pentanol respectively.

Further, the excess refractive index are fitted to Redlich – Kister polynomial equation of the form

$$Y^E = x_1(1-x_1)\sum_{i=0}^{n} a_i(1-2x_1)^i \qquad (2)$$

using least-squares regression method, the a_i coefficients are obtained by fitting above equation to the experimental values. The optimum number of coefficients is ascertained from an examination of the variation in standard deviation (σ)

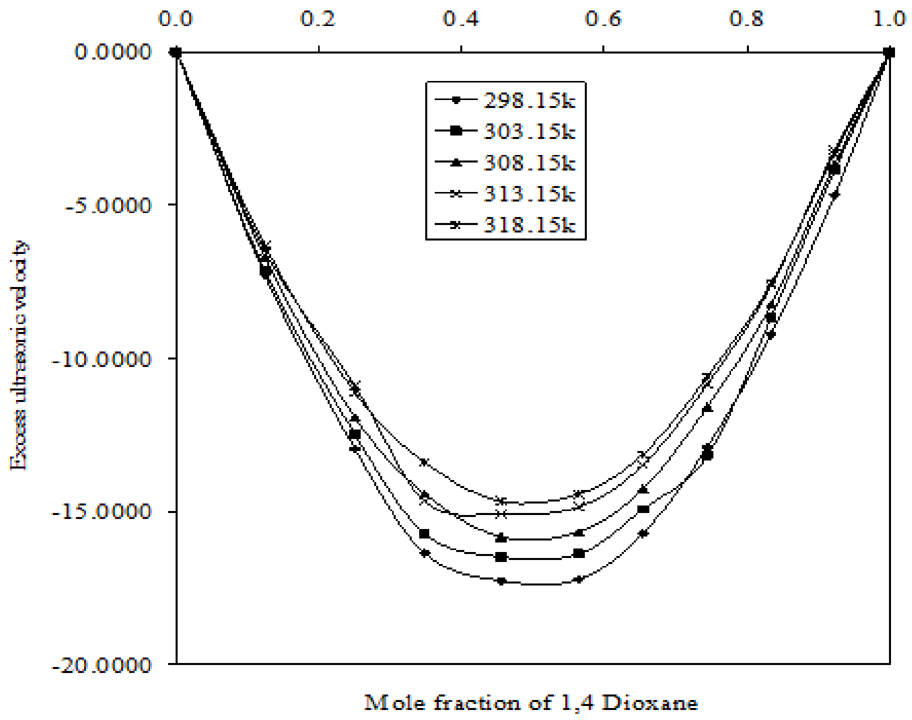
$$\sigma = \left[\frac{\sum (Y_{\exp t} - Y_{calc})^2}{N-n}\right]^{1/2} \qquad (3)$$

where N is the number of measurements, n is the number of coefficients. The values of coefficients, a_i and the standard deviations, σ are presented in Table 4.

Table -2: Ultrasonic speeds, Excess ultrasonic speeds and different theories at different temperatures

Experimental Values			Theoretical Values				
X_1	U_{Exp}	U^E	u_N	U_{IMP}	U_{Van}	U_R	U_{JR}
298.15K							
0.0000	1275.8	0.0000	1275.8	1275.8	1275.8	1275.8	1275.8
0.1235	1277.0	-7.2753	1282.6	1286.2	1283.7	1277.4	1292.5
0.2500	1280.0	-12.9524	1289.9	1296.1	1291.9	1282.2	1309.1
0.3476	1283.3	-16.3399	1295.9	1303.4	1298.4	1281.7	1320.2
0.4549	1289.7	-17.2583	1302.7	1311.0	1305.6	1289.2	1331.9
0.5645	1297.3	-17.2053	1310.2	1318.4	1313.1	1297.2	1341.6
0.6542	1304.9	-15.7174	1316.6	1324.1	1319.4	1304.4	1347.5
0.7446	1313.9	-12.8872	1323.3	1329.7	1325.7	1313.5	1351.0
0.8342	1323.7	-9.2028	1330.3	1335.0	1332.2	1324.0	1351.8
0.9228	1334.3	-4.6653	1337.6	1340.0	1338.6	1336.4	1349.4
1.0000	1344.3	0.0000	1344.3	1344.3	1344.3	1344.3	1344.3
RMSD			**0.6997**	**1.1463**	**0.8588**	**0.0822**	**2.3701**
303.15K							
0.0000	1258.9	0.0000	1258.9	1258.9	1258.9	1258.9	1258.9
0.1235	1259.6	-7.1357	1265.2	1268.5	1266.3	1260.0	1275.1
0.2500	1262.3	-12.4774	1272.0	1277.7	1273.9	1264.1	1291.0
0.3476	1265.3	-15.7069	1277.5	1284.5	1279.9	1263.2	1301.6
0.4549	1271.3	-16.4781	1283.9	1291.5	1286.6	1270.2	1312.8
0.5645	1278.4	-16.3762	1290.8	1298.3	1293.6	1277.7	1321.9
0.6542	1285.5	-14.9209	1296.7	1303.6	1299.3	1284.4	1327.2
0.7446	1293.0	-13.1698	1302.9	1308.8	1305.2	1293.0	1330.3
0.8342	1303.2	-8.6585	1309.4	1313.7	1311.2	1303.0	1330.6
0.9228	1313.6	-3.8388	1316.2	1318.4	1317.1	1315.0	1327.7
1.0000	1322.3	0.0000	1322.3	1322.3	1322.3	1322.3	1322.3
RMSD			**0.6925**	**1.1093**	**0.8442**	**0.0830**	**2.3670**
308.15K							
0.0000	1242.2	0.0000	1242.2	1242.2	1242.2	1242.2	1242.2
0.1235	1242.7	-6.7135	1247.9	1251.0	1248.9	1242.6	1257.7
0.2500	1244.8	-11.9174	1254.2	1259.4	1256.0	1246.2	1273.0
0.3476	1248.0	-14.4048	1259.3	1265.6	1261.5	1244.7	1283.1
0.4549	1252.9	-15.8153	1265.2	1272.1	1267.7	1251.4	1293.7
0.5645	1259.4	-15.6609	1271.5	1278.4	1274.1	1258.3	1302.2
0.6542	1266.1	-14.2637	1276.9	1283.3	1279.4	1264.5	1307.0
0.7446	1274.0	-11.5770	1282.7	1288.0	1284.8	1272.7	1309.6
0.8342	1282.6	-8.2342	1288.7	1292.6	1290.3	1282.2	1309.5
0.9228	1292.4	-3.6377	1294.9	1296.9	1295.7	1293.6	1306.2
1.0000	1300.5	0.0000	1300.5	1300.5	1300.5	1300.5	1300.5
RMSD			**0.6671**	**1.0541**	**0.8111**	**0.1129**	**2.3454**

Experimental Values			Theoretical Values				
X_1	U_{Exp}	U^E	u_N	U_{IMP}	U_{Van}	U_R	U_{JR}
313.15K							
0.0000	1225.5	0.0000	1225.5	1225.5	1225.5	1225.5	1225.5
0.1235	1225.6	-6.4816	1230.7	1233.5	1231.7	1225.4	1240.5
0.2500	1227.9	-10.8874	1236.4	1241.2	1238.1	1228.2	1255.1
0.3476	1229.3	-14.6493	1241.1	1246.8	1243.2	1226.3	1264.7
0.4549	1234.5	-15.0832	1246.4	1252.7	1248.8	1232.4	1274.7
0.5645	1240.6	-14.8501	1252.2	1258.4	1254.6	1238.8	1282.5
0.6542	1246.7	-13.4694	1257.1	1262.9	1259.4	1244.6	1286.8
0.7446	1254.2	-10.8456	1262.4	1267.2	1264.3	1252.3	1288.9
0.8342	1262.1	-7.6198	1267.8	1271.3	1269.3	1261.3	1288.3
0.9228	1271.3	-3.1951	1273.4	1275.3	1274.2	1272.1	1284.6
1.0000	1278.6	0.0000	1278.6	1278.6	1278.6	1278.6	1278.6
RMSD			**0.6570**	**1.0117**	**0.7921**	**0.1236**	**2.3384**
318.15K							
0.0000	1208.9	0.0000	1208.9	1208.9	1208.9	1208.9	1208.9
0.1235	1208.5	-6.3150	1213.7	1216.2	1214.5	1208.2	1223.3
0.2500	1209.9	-11.0999	1218.9	1223.2	1220.4	1210.5	1237.4
0.3476	1212.3	-13.3836	1223.1	1228.3	1225.1	1208.2	1246.5
0.4549	1216.3	-14.6551	1228.0	1233.7	1230.2	1213.9	1255.9
0.5645	1221.8	-14.4289	1233.3	1238.9	1235.5	1219.8	1263.2
0.6542	1227.5	-13.1265	1237.8	1243.0	1239.9	1225.2	1267.1
0.7446	1234.4	-10.5979	1242.6	1247.0	1244.4	1232.4	1268.8
0.8342	1241.8	-7.5409	1247.5	1250.7	1248.9	1241.0	1267.7
0.9228	1250.3	-3.3093	1252.7	1254.3	1253.4	1251.3	1263.7
1.0000	1257.3	0.0000	1257.3	1257.3	1257.3	1257.3	1257.3
RMSD			**0.6575**	**0.9847**	**0.7847**	**0.1512**	**2.3434**



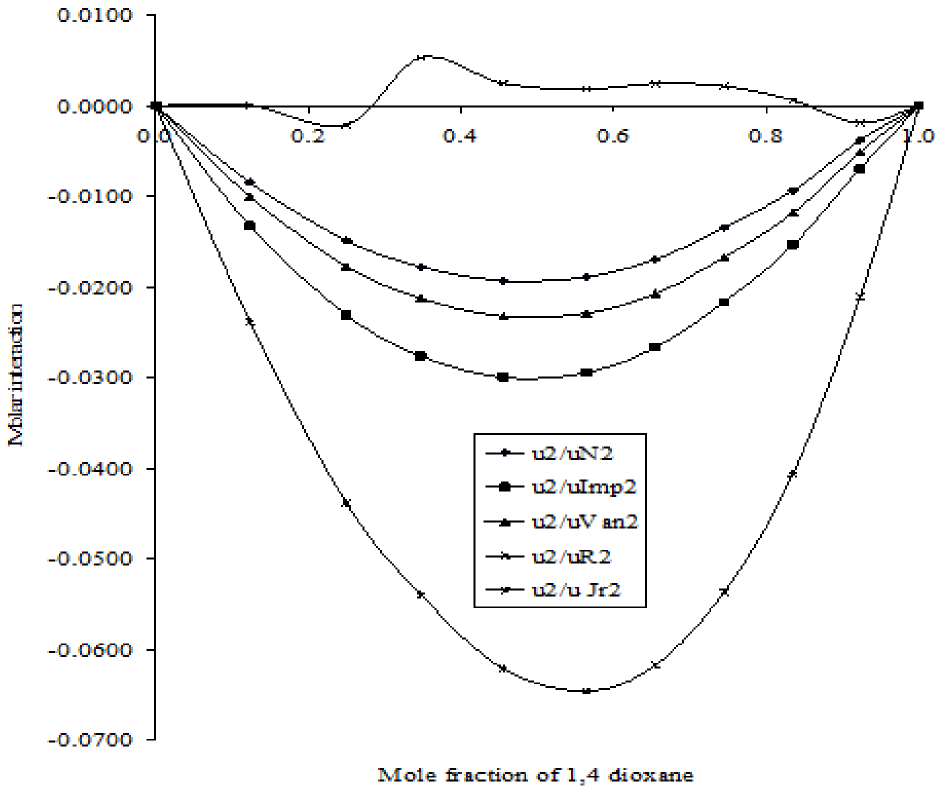
Variation Excess ultrasonic velocity with mole fraction of 1,4 DO at temperature range of 298.15 to 318.15 K in the system 1,4 DO + Pentanol

Table -3:- Molecular interaction parameter (α) for different theories at different temperatures

X_1	u_N	U_{IMP}	U_{Van}	U_R	U_{JR}	u_N	U_{IMP}	U_{Van}	U_R	U_{JR}
298.15K						**313.15K**				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1235	-0.0087	-0.0142	-0.0104	-0.0007	-0.0239	-0.0084	-0.0128	-0.0099	0.0003	-0.0239
0.2500	-0.0153	-0.0248	-0.0184	-0.0035	-0.0440	-0.0138	-0.0214	-0.0165	-0.0006	-0.0430
0.3476	-0.0193	-0.0306	-0.0232	0.0024	-0.0552	-0.0189	-0.0279	-0.0222	0.0048	-0.0552
0.4549	-0.0199	-0.0322	-0.0242	0.0007	-0.0624	-0.0190	-0.0288	-0.0227	0.0035	-0.0620
0.5645	-0.0196	-0.0317	-0.0240	0.0000	-0.0651	-0.0184	-0.0281	-0.0222	0.0028	-0.0643
0.6542	-0.0176	-0.0288	-0.0218	0.0007	-0.0622	-0.0165	-0.0254	-0.0201	0.0034	-0.0614
0.7446	-0.0142	-0.0236	-0.0178	0.0007	-0.0542	-0.0130	-0.0205	-0.0161	0.0030	-0.0533
0.8342	-0.0099	-0.0168	-0.0126	-0.0004	-0.0411	-0.0089	-0.0144	-0.0112	0.0013	-0.0402
0.9228	-0.0049	-0.0085	-0.0064	-0.0031	-0.0222	-0.0034	-0.0063	-0.0046	-0.0013	-0.0207
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
303.15K						**318.15K**				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1235	-0.0088	-0.0140	-0.0105	-0.0006	-0.0241	-0.0085	-0.0125	-0.0099	0.0005	-0.0240
0.2500	-0.0152	-0.0240	-0.0182	-0.0029	-0.0440	-0.0147	-0.0217	-0.0172	-0.0011	-0.0439
0.3476	-0.0191	-0.0297	-0.0228	0.0033	-0.0551	-0.0176	-0.0259	-0.0207	0.0068	-0.0540
0.4549	-0.0195	-0.0310	-0.0237	0.0017	-0.0622	-0.0191	-0.0281	-0.0225	0.0038	-0.0621
0.5645	-0.0192	-0.0305	-0.0234	0.0010	-0.0648	-0.0185	-0.0275	-0.0221	0.0033	-0.0645
0.6542	-0.0172	-0.0277	-0.0212	0.0017	-0.0619	-0.0167	-0.0249	-0.0200	0.0037	-0.0616
0.7446	-0.0152	-0.0240	-0.0187	-0.0001	-0.0553	-0.0132	-0.0201	-0.0161	0.0032	-0.0535
0.8342	-0.0096	-0.0160	-0.0122	0.0002	-0.0408	-0.0092	-0.0143	-0.0114	0.0013	-0.0405
0.9228	-0.0039	-0.0073	-0.0053	-0.0021	-0.0212	-0.0038	-0.0064	-0.0049	-0.0017	-0.0210
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
308.15K										
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000					
0.1235	-0.0085	-0.0133	-0.0100	0.0000	-0.0239					
0.2500	-0.0149	-0.0231	-0.0177	-0.0021	-0.0438					
0.3476	-0.0178	-0.0276	-0.0213	0.0053	-0.0540					
0.4549	-0.0193	-0.0300	-0.0232	0.0025	-0.0621					
0.5645	-0.0189	-0.0294	-0.0229	0.0019	-0.0646					
0.6542	-0.0170	-0.0267	-0.0207	0.0024	-0.0617					
0.7446	-0.0135	-0.0217	-0.0167	0.0021	-0.0537					
0.8342	-0.0094	-0.0154	-0.0118	0.0006	-0.0407					
0.9228	-0.0038	-0.0070	-0.0051	-0.0019	-0.0211					
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000					

Table 4. Coefficients (a_i) and standard deviation (σ) for 1,4 Dioxane + 1-Pentanol

Property	T/K	a_0	a_1	a_2	a_3	a_4	σ *100
	298.15	-70.3169	-3.1928	4.1178	4.6591	4.8571	0.1801
	303.15	-66.4616	-0.1839	-14.8127	-5.0176	38.6842	0.3051
U^E	**308.15**	-63.6781	-0.4551	2.2635	-6.3786	10.6947	0.0970
	313.15	-61.3432	-3.5082	6.5861	-2.0703	9.5719	0.3884
	318.15	-58.8706	-1.3704	2.3725	-6.0947	8.8995	0.0973



V ariation molar interaction with different theories at temperature 308.15K in the binary system 1,4 dixoane + Pentanol

RESULTS AND DISCUSSION

The experimental values of ultrasonic speeds (U), says that at each temperature as mole fraction of 1, 4 dioxane increases the ultrasonic speeds of the binary increases. Also the data of Table 2 shows at each concentration, as temperature increases ultrasonic velocity decreases as reported by several researchers [17, 18], G. R.Bedare et al studied molecular interactions in the binary mixtures 1, 4 dioxane with ethanol and methanol and they reported, as ultrasonic speeds of the mixture increases with concentration of 1, 4 dioxane in both the binaries indicates the presence of strong molecular interaction. Similar like reported are made by the author in their earlier paper [19] on 1-butanol with hexane.

Using empirical relations viz., Nomoto, Impedance, Van dael, Rao's specific velocity and Junjie's ultrasonic speeds are elevated and reported in Table 2. The close inspection of this table shows good agreement with the Rao's specific sound velocity followed by Nomoto's, Van dael, Impedance and Jungie's realtions with experimental values. We also report the root mean square deviation for the above theories. It is a well known fact that, the molecular interaction parameters (α) is used to understand different kinds of association, molecular packing and various types of intermolecular interactions and their strength of influence by the size of pure components and their mixture. The evaluated values of 'α' at different temperatures are presented in the Table 3, and plots are observed at 308.15K as shown in Fig.2, similar trends observed at rest of the temperatures. All these values are found to be negative and shows presence of strong interactions. The same is conformed with negative excess ultrasonic speeds reported in table 2 at different temperatures. Similar like reports are made by Shashi Singh *et al* [20], there plots are presented in Fig. 1. At the end , the respective coefficients (a_i) of U^E and standard deviation (σ) for the chosen binary are reported in Tables 5. The values of coefficients, a_i, were evaluated by using the method of least-squares with all points weighted equally.

CONCLUSION

The theoretical evaluations of ultrasonic speeds with binary liquid mixture are determined, and the validity of different theories is checked. The study gives satisfactory results with all the theories and it is observed that out of all the theories Rao's specific sound velocity realtion gives best suited followed by Nomoto's, Van dael, Impedance and Jungie's realtions. The negative values of impact parameter and excess ultrasonic speeds reflects the existence of strong specific inter molecular interactions in the binary mixture.

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