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RESEARCH ARTICLE

Theoretical Evaluation of Ultrasonic Velocities in Ternary Liquid Mixture at Different Temperatures

S. BALAKRISHNAN[1*] and R. PALANI[2]

[1]Department of Physics, Achariya College of Engineering Technology,
Puducherry- 605110, India

[2]Department of Physics, DDE, Annamalai University, Tamilnadu, India

bala.phy@gmail.com

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Abstract: Theoretical values of ultrasonic velocity in the ternary mixtures of diisopropylether+2,2,2-trifluoroethanol+1-propanol have been evaluated at temperatures 303 K, 308 K and 313 K using Nomoto's Relation (U_{NR}), Junjie's Method (U_{JM}), Ideal Mixing Relation (U_{IMR}), Free Length Theory (U_{FLT}), Collision Factor Theory (U_{CFT}) and Impedance Dependence Relation (U_{IDR}). Theoretical values were compared with the experimental values and the validity of the theories was checked by calculating the average percentage error (APE).

Keywords: Ultrasonic velocity, Collision factor theory, Ternary liquid mixtures, Average Percentage Error

Introduction

Ultrasonic velocity of sound waves in a medium is fundamentally related to the binding forces between the molecules. Ultrasonic velocities of the liquid mixtures consisting of polar and non-polar components are of considerable importance in understanding intermolecular interaction between component molecules and find application in several industrial and technological process[1]. Several researchers[2-5] carried out ultrasonic investigations and correlated the experimental results of ultrasonic velocity with the theoretical relations of Nomoto[6], Junjie[7], Van Deal and Vangeel[8], Jacobson[9], Schaaf[10] and Impedance dependence relation[11]. In the present communication the aforementioned relations have been used to predict ultrasonic velocity in ternary liquid mixtures of diisopropylether+2,2,2-trifluoroethanol+1-propanol at 303,308 and 313 K.

Experimental

All the chemical used were of analytical reagent (AR) and spectroscopic reagent (SR) without further purification. The purities of the above chemicals were checked by density determination at 303, 308 and 313±0.1 K, which showed an accuracy of $\pm 1\times10^{-4}$ gcm^{-3}. The ternary liquid mixtures of different known compositions were prepared in stopper measuring flasks. The density, viscosity and velocity were measured as a function of composition of the ternary liquid mixture at 303, 308 and 313 K for mixed solvent systems in which 1-propanol was added to a binary mixtures of diisopropylether and 2,2,2-tri-fluroethanol. For this purpose binaries with fixed volume ratios $X_1/X_2 \cong 4:1$ were prepared. The density was determined using a specific gravity bottle by relative measurement method with an accuracy of ±0.01 kgm^{-3}. The weight of the sample was measured using electronic digital balance with an accuracy of ±0.1 mg (Model: SHIMADZU AX-200). An ultrasonic interferometer having the frequency of 3 MHz (MITTAL ENTERPRISES, New Delhi, Model: F-81) with an overall accuracy of ±0.1% has been used for velocity measurement. An electronically digital operated constant temperature bath (RAAGA Industries) has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature. The accuracy in the temperature measurement is ±0.1 K.

Theory and calculations

Ultrasonic velocities were determined on the basis of different theories and relations as discussed earlier[12].

Results and Discussion

The values of ultrasonic velocities computed theoretically using the relations of Nomoto, Junjie, Van Dael and Vangeel, Jacobson’s Free Length Theory, Impedance Dependence Relation and Schaaf’s Collision Factor Theory together with experimental values for the ternary mixture of diisopropylether(x_1)+2,2,2-trifluoroethanol(x_2)+1-propanol(x_3) at the temperatures 303 K, 308 K and 313 K are presented in Table 1. The percentage deviation, Average Percentage Error (APE) of sound velocity using the above theory for the mixtures studied are given in Table 2.

Table 1. Experimental and theoretical values of ultrasonic velocity in diisopropylether (x_1)+2,2,2-trifluoroethanol (x_2)+1-propanol(x_3) (x_1/x_2=4:1) at 303, 308 and 313 K

Mole Fraction X_3	U_{EXP} ms^{-1}	U_{NR} ms^{-1}	U_{JM} ms^{-1}	U_{IMR} ms^{-1}	U_{FLT} ms^{-1}	U_{CFT} ms^{-1}	U_{IDR} ms^{-1}
			303 K				
0.0000	922.3	945.5	930.3	932.1	1006.9	969.2	922.2
0.0210	924.3	948.5	932.5	936.0	1024.1	981.8	927.8
0.0405	931.2	951.5	934.9	939.9	1048.8	997.4	933.3
0.0601	936.4	954.5	937.3	943.9	1071.0	1011.6	938.9
0.0802	941.5	957.7	939.7	948.0	1082.7	1021.1	944.6
0.0998	946.9	960.7	942.2	952.1	1093.1	1029.9	950.2
			308 K				
0.0000	918.8	922.9	907.0	908.8	1013.5	961.7	898.3
0.0210	920.0	925.7	909.1	912.6	1018.3	968.4	903.7
0.0405	921.4	928.5	911.2	916.4	1042.9	983.9	909.2
0.0601	925.2	931.4	913.4	920.2	1085.2	1006.6	914.7
0.0802	931.0	934.3	915.7	924.1	1092.5	1014.0	920.2
0.0998	943.5	937.1	918.0	928.0	1116.5	1028.1	925.7
			313 K				
0.0000	893.7	914.0	897.7	899.9	1008.0	955.3	889.1
0.0210	894.7	916.8	899.8	903.8	1034.9	972.2	894.8
0.0405	898.2	919.7	901.9	907.7	1043.0	980.4	900.4
0.0601	904.5	922.5	904.0	911.6	1072.9	998.0	906.1
0.0802	913.5	925.5	906.3	915.6	1095.5	1012.0	911.7
0.0998	923.5	928.4	908.6	919.7	1107.6	1021.4	917.4

Table 2. Percentage deviation and Average Percentage Error for the system diisopropylether (x_1)+2,2,2-trifluoroethanol (x_2)+1-propanol(x_3) (x_1/x_2=4:1) at 303, 308 and 313 K

Mole Fraction X_3	% U_{NR}	% U_{JM}	% U_{IMR}	% U_{FLT}	% U_{CFT}	% U_{IDR}
			303 K			
0.0000	-2.5172	-0.8640	-1.0582	-09.1753	-5.0894	0.0132
0.0210	-2.6143	-0.8915	-1.2630	-10.7982	-6.2185	-0.3735
0.0405	-2.1766	-0.3940	-0.9382	-12.6297	-7.1088	-0.2298
0.0601	-1.9362	-0.0913	-0.8061	-14.3753	-8.0262	-0.2713
0.0802	-1.7155	0.1909	-0.6915	-15.0027	-8.4510	-0.3244
0.0998	-1.4564	0.4951	-0.5518	-15.4375	-8.7634	-0.3465
APE	-2.0694	-0.2591	-0.8848	-12.9031	-7.2762	-0.2554
			308 K			
0.0000	-0.4503	1.2831	1.0863	-10.3117	-4.6732	2.2359
0.0210	-0.6184	1.1854	0.8082	-10.6803	-5.2564	1.7696
0.0405	-0.7699	1.1038	0.5474	-13.1838	-6.7845	1.3249
0.0601	-0.6652	1.2732	0.5408	-17.2988	-8.7984	1.1378
0.0802	-0.2975	1.6995	0.7961	-17.2813	-8.8543	1.2171
0.0998	0.6775	2.7052	1.6405	-18.3333	-8.9673	1.8907
APE	-0.3541	1.5417	0.9032	-14.5149	-7.2224	1.5960
			313 K			
0.0000	-2.2744	-0.4470	-0.6945	-12.7932	-6.8912	0.5121
0.0210	-2.5171	-0.6101	-1.0576	-15.7227	-8.7124	-0.0519
0.0405	-2.3881	-0.4087	-1.0529	-16.1218	-9.1514	-0.2464
0.0601	-1.9952	0.0507	-0.7856	-18.6195	-10.336	-0.1735
0.0802	-1.3137	0.7915	-0.2302	-19.9283	-10.785	0.1934
0.0998	-0.5282	1.6179	0.4168	-19.9366	-10.605	0.6600
APE	-1.8361	0.1657	-0.5673	-17.1872	-9.4137	0.1489

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 interactions between the components of liquid mixtures have been taken into account. The assumption for the 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 nonelastic 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.

It is observed from Table 2 that there is a good agreement between experimental and theoretical values calculated by Junjie's relation followed by Impedance dependence relation, Ideal mixing relation and Nomoto's relation while higher deviations are observed in CFT and FLT. 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 mixtures. Similar kinds of results were obtained by earlier workers[13-14]. The deviations between theoretical and experimental values of ultrasonic velocities decrease with increase of temperature due to breaking of hetero and homo molecular clusters at higher temperatures[15]. On increasing the temperature, the ultrasonic velocity values decrease in the ternary liquid mixture. This is probably due to the fact that the thermal energy activates the molecule, which would increase the rate of association of unlike molecules. The magnitude of APE is in order: JM<IDR<IMR<NR<CFT<FLT.

Conclusion

Ultrasonic velocities evaluated using NR, JM, IMR, FLT, CFT and IDR were compared with experimentally measured velocity values at temperatures 303 K, 308 K and 313 K for the studied ternary mixtures. It may be concluded that JM, IDR, IMR and NR relations are better suited for the ternary mixture at all temperatures. The observed deviation of theoretical values of velocity from the experimental values is attributed to the presence of intermolecular interactions in the system studied.

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