Molecular Interaction Studies on Binary Liquid Mixture Containing O-Cresol and Formamide at 318.15 K

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Abstract: Ultrasonic velocity, density and viscosity of binary liquid mixture containing O-Cresol and Formamide have been calculated as a function of mole fractions by using ultrasonic interferometer of frequency 2MHz at 318.15K. The change in adiabatic compressibility ($\Delta \beta_{ad}$), excess intermolecular free length (L_f^E) and excess free volume (V^E) have been calculated. Positive deviations of ultrasonic velocities and negative deviations of adiabatic compressibility from mole fraction mixture law have been observed. The observed variations of these parameters, with concentration and temperature, are discussed in terms of the intermolecular interactions between the unlike molecules of the binary mixtures.

Keywords: O-Cresol, Formamide, ultrasonic velocity, viscosity, density

1. Introduction

Intermolecular interactions play a vital role in liquid mixtures. They effect the arrangement, coordination and conformations of the molecules in solutions. Studies on density, ultrasonic velocity, viscosity, acoustic, thermodynamic, excess thermodynamic parameters and their deviations in binary systems have been the subject of many investigations in the recent years [1-7]. Rectilinear propagation is a characteristic exhibited by ultrasonic waves because of their short wavelength [8,9]. The short wavelength of the ultrasonic waves is the factor that has been made possible the application of these waves in many cases. These interactions can be explained on the basis of excess thermodynamic parameters [10-13]. By using the experimentally measured values of ultrasonic velocity (U), density (ρ) and viscosity (η) various excess parameters like change in adiabatic compressibility ($\Delta\beta_{ad}$), excess intermolecular free $length(L_f^E)$ and excess ultrasonic velocity(U^E) have been calculated for the liquid mixture. There is continuing need for reliable thermodynamic data of binary systems for chemical industries as the data is essential in the design of processes involving chemical separation, heat transfer, mass transfer and fluid flow.

2. Materials and Experiments

All the materials procured of Sigma-Aldrich AR grade and glassware used of Borosilicate make. Organic liquid O-Cresol, Formamide of AR grades were procured from Sigma-Aldrich are used directly without purification. The densities and viscosities of the liquid compounds were measured with specific gravity bottle and Ostwald viscometer pre calibrated with 3D [14] water of Millipore to nearest mg/ml. The time taken for flow of viscous fluid in Ostwald viscosity meter is measured to a nearest 0.01 sec. Borosilicate glassware, Japan make Shimadzu electronic balance of sensitivity +0.001gm and constant temperature water bath of accuracy +0.1K were used while conducting the experiments. 2MHz ultrasonic interferometer model no.

F-05 with least count of micrometer 0.001mm of Mittal Enterprises [15] was used for calculating velocities of sound waves and all the tests were conducted as per ASTM standard [16] procedures.

3. Theory

In order to examine the inter molecular interactions in liquid mixtures of O-Cresol and Formamide, experiments were conducted to find the density, viscosity and velocity of 2MHz ultrasonic waves for pure liquids and for binary liquid mixtures. From the experimental data of binary mixtures, the derived, excess values were calculated at various mole fractions of o-cresol for understanding inter and intra molecular interactions at 318.15K temperature. The derived and excess values are calculated by using the fallowing relations adiabatic compressibility (β_{ad}), Intermolecular free length (L_f) free volume and viscosity of the binary liquid mixture. But on mixing two liquids, the interaction between the molecules of the two liquids takes place because of the presence of various types of forces such as dispersive forces, charge transfer, hydrogen bonding, dipole-dipole and dipoleinduced dipole interactions.

Table 1: The values of density (ρ), ultrasonic velocity (U),viscosity (η), adiabatic compressibility (β_{ad}), free volume(V) and intermolecular free length (L_f) along with molefraction of O-Cresol with Formamide.

Х	U	Р	η	β_{ad}	L _f	V
0.0000	1557.10	1.1179	1.9691	36.8947	0.3890	40.2898
0.0409	1553.65	1.1124	2.4000	37.2421	0.3909	42.8106
0.0876	1548.81	1.1070	2.8700	37.6579	0.3930	45.6801
0.1413	1542.44	1.1015	3.4000	38.1593	0.3957	48.9861
0.2038	1534.34	1.0958	3.9400	38.7648	0.3988	52.8422
0.2775	1524.80	1.0890	4.4300	39.4940	0.4025	57.4354
0.3655	1513.30	1.0810	4.8900	40.3939	0.4071	63.0002
0.4726	1499.64	1.0709	5.1909	41.5218	0.4127	69.9057
0.6057	1482.87	1.0581	5.3800	42.9810	0.4199	78.6904
0.7756	1461.37	1.0426	5.4000	44.9120	0.4292	90.1415
1.0000	1432.10	1.0241	5.4120	47.6114	0.4420	105.595

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Figure 1-4: Viscosity (η), adiabatic compressibility (β_{ad}), free volume (V) and intermolecular free length (L_f) along with mole fraction of O-Cresol

 Table 2: The excess parameter of adiabatic compressibility, intermolecular free length, free volume and viscosity along with mole fraction of O-Cresol with Formamide

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Х	$\Delta \beta_{ad}$	η	L _f ^E	V ^E
0.0000	0.0000	0.0000	0.0000	0.0000
0.0409	-0.0912	0.2900	-0.0003	-0.1520
0.0876	-0.1756	0.5993	-0.0006	-0.3308
0.1413	-0.2500	0.9443	-0.0008	-0.5336
0.2038	-0.3145	1.2691	-0.0010	-0.7600
0.2775	-0.3745	1.5055	-0.0012	-0.9760
0.3655	-0.4180	1.6625	-0.0013	-1.1600
0.4726	-0.4378	1.5946	-0.0013	-1.2484
0.6057	-0.4050	1.3255	-0.0012	-1.1560
0.7756	-0.2947	0.7605	-0.0009	-0.8000
1.0000	0.0000	0.0000	0.0000	0.0000



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Figures 5-8: Adiabatic compressibility, intermolecular free length, free volume and viscosity along with mole fraction of O-Cresol

4. Results and Discussion

Values of density (ρ), ultrasonic velocity (U), viscosity (η), adiabatic compressibility (β_{ad}), free volume (V) and intermolecular free length (L_f) along with mole fraction of O-Cresol with Formamide are listed in the table (1). The excess parameter of adiabatic compressibility, intermolecular free length, free volume and viscosity along with mole fraction of O-Cresol with Formamide listed in table (2). Also the graphical representation for above said parameter against mole fraction (X) of O-Cresol is depicted from the figures 1 to 8. Ultrasonic velocity in medium is depends upon binding forces between the molecules. From the table (1) it is clear that in the system O-Cresol with Formamide the ultrasonic velocity decreases with increasing mole fractions of O-Cresol. The decrease in velocity and increase in compressibility were attributed to the formation of hydrogen bonds between solute and solvent molecules [17]. From table (2), the negative values of excess parameters shows there is weak molecular interaction existing between unlike molecules [18]. The excess intermolecular free lengths are negative. It shows sound waves cover long distance due to decrease in intermolecular free length. It means dominant nature of hydrogen bond interaction between unlike molecules [19]. The excess value of adiabatic compressibility, inter molecular free length and free volumes, all are negative value indicates the weak molecular interaction between unlike molecules of components liquid.

5. Conclusions

The ultrasonic velocity, density, viscosity and other related experimental, derived and their excess parameters were calculated. The miscible organic binary liquid mixture of O-Cresol with Formamide shows the negative excess free volume (V^E) and positive excess viscosity (η) represent the strong interaction between the unlike molecules of the binary mixture.

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