Vol 5, Issue 8, 2022 **Impact Factor:2.58** DOI: https://doi.org/10.31426/ijamsr.2022.5.8.5611

IJAMSR

International Journal of Advanced Multidisciplinary Scientific Research (IJAMSR) ISSN:2581-4281

Comparative Study Of Molecular Interaction In Associated Liquids

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A B S T R A C T

The ultrasonic studies in solutions are of great use in understanding the nature and strength of molecular interaction. The thermo-physical parameters like ultrasonic velocity, relative density and relative viscosity, refractive index have been measured for the pure state of tetrahydrofuran and m-cresol at different temperatures at 2MHz frequencies. The experimental data of ultrasonic velocity, density, viscosity and refractive index have been used for the comparative study of molecular interaction in the pure state of tetrahydrofuran (C4H8O) and m-cresol at 200C, 300C, 400C indicative of the nature of interaction between them.

Keywords: Density, Viscosity, Ultrasonic Velocity, Refractive Index, Molecular interaction.

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1. Introduction

In recent years ultrasonic technique has become a powerful tool in providing information regarding the molecular behavior of liquids. Ultrasonic velocity is associated with binding forces between atoms and molecules, which is highly sensitive in molecular interaction and consequently employed in studying nature and strength of molecular interaction in the solutions. Variation of ultrasonic velocity and associated acoustical parameters furnish information about velocity and structural changes due to weakly and strongly interacting components of the solutions. Ultrasonic technology is employed in medicine, biology, industry, material science, agricultural, oceanography, dentistry, consumer industry, sonochemistry research etc. Due to its non destructive nature, it is extensively used in understanding the structures of the polymers and also furnishes knowledge on solvophilic or solvophobic nature of polymers.

Ultrasonic Characterization is a versatile sensitive non destructive tool, to explore not only the micro structural state of the material, but also to derive information about the defect state of material.

Ultrasonic technique is a powerful tool for material characterization due to the well developed basic understanding of the ultrasonic wave propagation availability of the wide frequency ranges for the interaction if ultrasonic waves with microscopic and macroscopic structural features with different scattering and absorption mechanisms lattice defects etc. The measurements are temperature dependent ultrasonic longitudinal velocities in materials have been used to explore the physicochemical properties, structural/phase changes, charge ordering, curie temperature, Jhan teller temperature, phase transition temperature. The first differentials of the temperature dependent ultrasonic parameter have been used as an effective tool to identify the structural/micro structural change in the materials.

Measurements

Density (ρ), viscosity (η), ultrasonic velocity (U) and refractive index (nD) measurements on pure polar solvents. Pure Tetra-hydro furan (THF) (C4H8O) and m-cresol solutions were carried out at 20°C, 30°C, 40°C.The ultrasonic speeds (U) in pure liquids were measured by using a single crystal variable path ultrasonic.

Interferometer operating at 2-MHz. The ultrasonic speeds were reproducible within ms-1. The densities (ρ) of pure liquids were measured by using a single-capillary pycnometer made of borosil glass having a bulb capacity of 8 x 10-6 m3. The capillary with graduated marks, had a uniform bore and could be closed were calibrated by using triple distilled water. The reproducibility in relative density measurement was within kgm-3. Refractive index can be measured easily with a high degree of accuracy at constant temperature and wavelength of light used. Refractive indices were measured

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with calibrated and thermostats of Abbe's refractometer, using D-line of sodium as the source of light. The instrument was calibrated with the help of a piece of glass of known refractive index (at 250C nD=1.1519) provided with the instrument.

Result And Discussion

The experimental values of ultrasonic velocity (U), density (ρ), viscosity (η) Refractive Index (nD) of pure liquids of Tetrahydrofuran (THF) and m-cresol solutions were carried out at 20°C, 30°C, 40°C are reported in Table-1.

Temperature ^{0}C	Ultrasonic Velocity (U) (m/sec.)		Relative Density (P) (Kgm/m^3)		Relative Viscosity (η) (c-Poise)		Refractive Index (n_D)	
	C_4H_8O	m-cresol	C_4H_8O	m-cresol	C_4H_8O	m-cresol	C_4H_8O	m-cresol
20	1240.00	1504.5	0.895	0.977	0.952	1.085	1.406	1.538
30	1250.23	1467.0	0.888	0.969	1.124	0.568	1.403	1.535
40	1150.00	1435.6	0.882	0.960	1.034	0.528	1.398	1.532

Table 1: Comparison of experimental values of ultrasonic velocity (U), density (ρ) and viscosity (η) of pure state of tetrahydrofuran and m-cresol at different temperature.

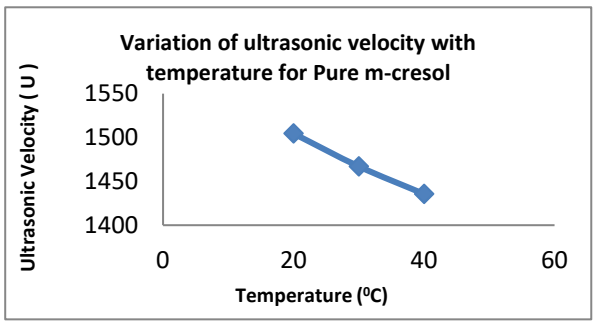

Figure-1

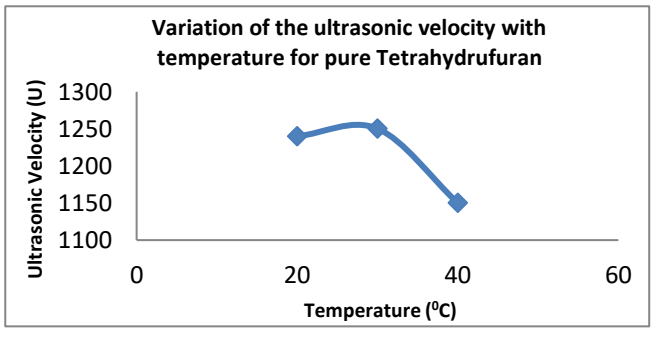

Figure-2

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Figure 1 & 2: shows that the plot of experimental ultrasonic velocity versus different temperatures 200C, 300C, 400C. It is observed that the ultrasonic velocity increases with increase in temperature in case of pure m-cresol. It is also clearly seen that smaller the temperature, greater the ultrasonic incase of pure m-cresol, indicating the more stability of polar molecules. But in case of pure tetrahydrofuran shows opposite and non linear variation of ultrasonic velocity. In pure tetrahydrofuran ultrasonic velocity decreases with increase in temperature shows strongly supports the presence of intermolecular interactions through hydrogen bonding.

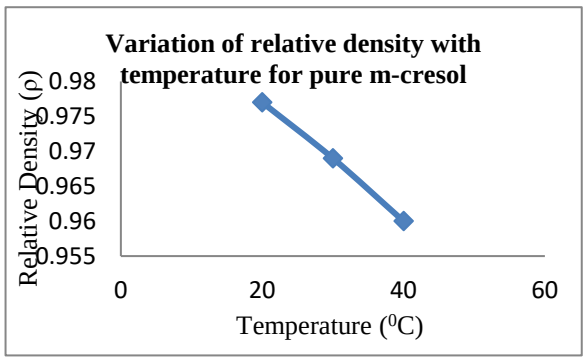

Figure-3

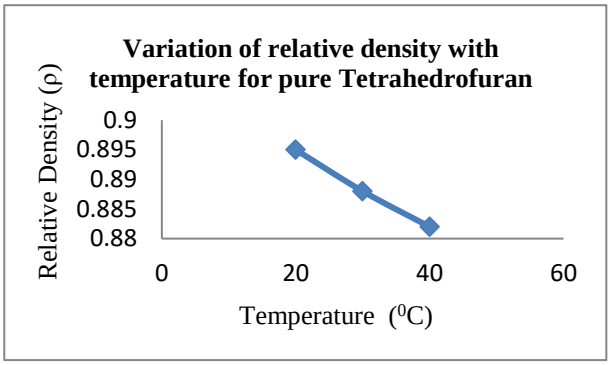

Figure-4

Figure 3 & 4: shows that the plot of experimental relative density of pure tetrahydrofuran and pure p-cresol at different temperatures 200C, 300C, 400C. It is observed that the relative density decreases with increase in temperature in case of pure tetrahydrofuran and m-cresol. The variation of these properties with temperature and composition for containing polar molecules and hydrogen bonded components may be complex due to a decrease or an increase in hydrogen bonding interaction. Depending on the nature of the liquids whether they are polar or non-polar. The relative density and the volume can throw light on the strength of the interactions. The decrease in relative density with increase in temperature indicates the tendency of the system towards ideal behavior.

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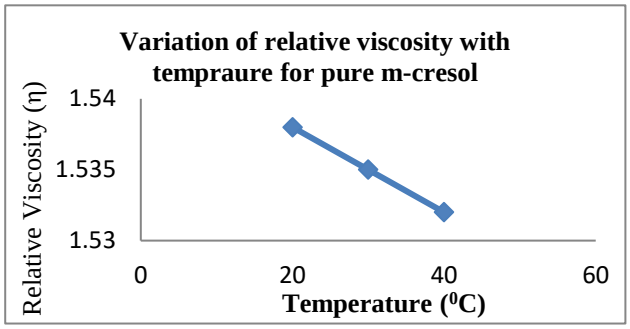

Figure-5

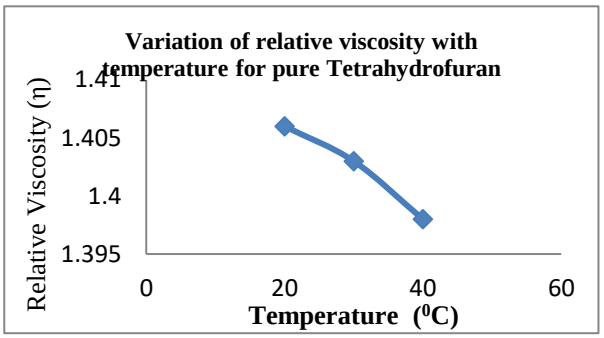

Figure-6

Figure 5 & 6: shows that the plot of experimental relative viscosity at different temperatures 200C, 300C, 400C. It is observed that the relative viscosity increases with increase in temperature in case of pure tetrahydrofuran but in case of m-cresol relative viscosity decreases with increase in temperature. The decreases in viscosity in the vicinity of the isotropic transition due to the transition from the disordered isotropic liquid phase to the molecules tend to align parallel to each other. In case of tetra hydro furan relative viscosity increase with increase of temperature due to it intermolecular distance increases and hence increases in close packing of the molecule.

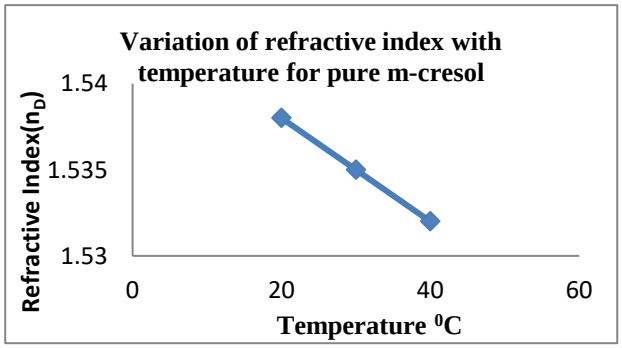

Figure- 7

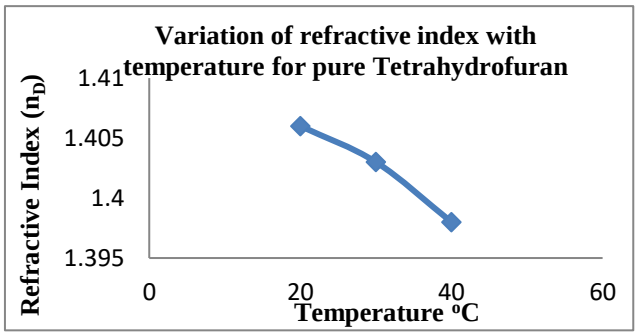

Figure-8

Figure-7 & 8: shows that the plot of experimental refractive index at different temperature 200C, 300C, 400C. It is observed that the refractive index decreases with increase in temperature in case of pure tetrahydrofuran and pure p-cresol is shows that tetrahydrofuran and p-cresol find the associative behavior of the liquid.

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Conclusion

The experimental study of Ultrasonic velocity, density, viscosity and refractive index between 200C to 400C shows that m-cresol find the associative behavior of the liquid. The comparative study of m-cresol and Tetrahydrofuran gives the very fruitful information about the molecular interaction and induction forces. The relative viscosities of m-cresol and tetrahydrofuran shows opposite nature with respect to temperature due to molecules are densily packed in the liquid state. The temperature variation significantly affects the bulk properties of the material and is close with the theory. The linear behaviors of both the liquids are due to associativeness of the molecules of the system.

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