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Molecular interaction study of linoleic acid with α-tocopherol by ultrasonic technique

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ABSTRACT

Ultrasonics has become an important and powerful research tool in physics. The ultrasonic study of liquid mixtures has been gaining importance in assessing the nature of molecular interactions and understanding the physico-chemical behaviour of liquid. In present investigation, ultrasonic velocity, density, viscosity has been measured in liquid mixture of linoleic acid (9, 12-Octadecadienoic acid) and α-tocopherol (Vitamin E) with different compositions using ethanol as solvent. The measurements are done at 2MHz frequency and in temperature range 293K to 313K using pulse echo technique. Thermo acoustical parameters viz., adiabatic compressibility, relaxation time, free length, acoustic impedance, and internal pressure have been computed from the experimental data. The variation of ultrasonic velocity and other thermo-acoustical parameters shows nonlinear increase or decrease with variation in composition. The nature of solute-solute and solute-solvent interactions and effect of composition on molecular interactions have been studied.

Keywords: Linoleic acid, α-tocopherol, pulse echo technique.

INTRODUCTION

Carbonyl (aldehyde) group and hydroxyl (-OH) group are the part of several biologically important molecules such as proteins, amino acids, lipids, peptides. These groups can interact with basic ,acidic and other functional groups present in biological system to form complexes either by chemical bonding or hydrogen bonding and affect the properties of biomolecules[1]. Literature survey reveals that ultrasonic, volumetric, viscometric study is done on biomolecules like proteins, amino acids, peptides[2-5]. Biomolecules called lipids are naturally occurring organic compounds commonly known as oils and fats. Linoleic acid (9, 12-Octadecadienoic acid) is unsaturated omega-6-fatty acid which is essential fatty acid for human body. α-tocopherol is fat soluble antioxidant and protects retina from glaucomatous damage. Ultrasonic, viscometric study is already done on linoleic acid with certain drugs [6-7]. This paper divulges molecular mechanism of linoleic acid with α-tocopherol (Vitamin-E) in solvent ethanol by measurement of thermo acoustical parameters.

MATERIALS AND METHODS

Master solutions have been prepared by dissolving 1gm of each solute in 100 ml ethanol separately in air tight bottles at room temperature. After this compositions of LA/TOCO are prepared in ratios (100/0, 80/20, 60/40, 40/60, 20/80, 0/100) taking appropriate amount from stock solution.

Ultrasonic Velocity measurement is done by MHF-400 high frequency pulser receiver (supplied by Roop Telsonic ultrasonix Ltd). Ultrasonic pulser receiver is advanced technique which provides unique low cost ultrasonic measurement capability. The instrument has spike pulser and broadband receiver. The receiver has max gain of 103dB, adjustable in minimum step of 1dB. 4 high pass and low pass filters each facilitate frequency cut off for optimization of received signal.

The ultrasonic velocity measurement is done at 2MHz frequency and at temperatures 293K, 298K, 303K, 308K, 313K for LA/TOCO compositions.

The densities of all compositions have been measured by pycnometer at temperatures 293K, 298K, 303K, 308K, 313K.The viscosity measurement is done by Ostwald's Viscometer.

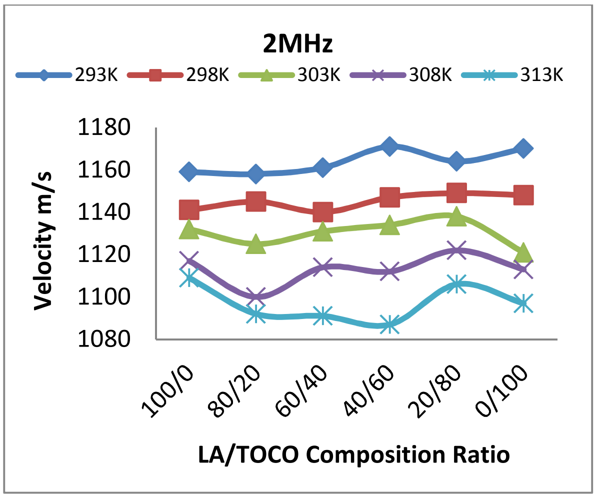
Ultrasonic velocity, density and viscosity measurements change even with very small change of temperature. Therefore for such measurements it is very necessary to keep temperature constant accurately. Plasto craft thermostat (LTB -10) maintains desired accurate constant temperature with accuracy of $\pm 0.1^0$C in temperature range -10^0C to 95^0C.

THEORETICAL FORMULATIONS

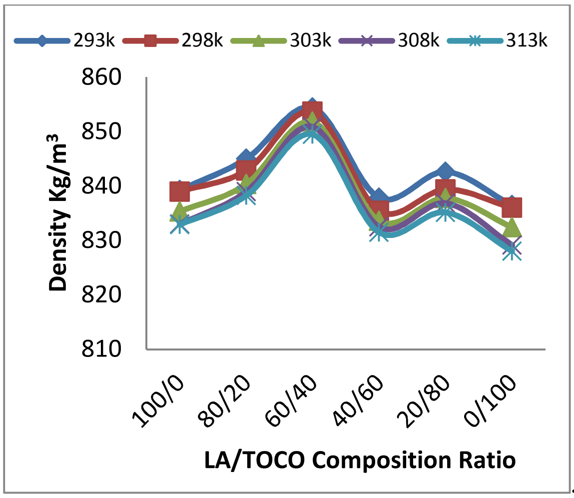
1. Ultrasonic velocity $\boldsymbol{u} = \frac{\boldsymbol{2d}}{\boldsymbol{t}}$ …. m/sec
2. Density $\rho = (\frac{M_l}{M_w})\rho_w$ ….Kg/m^3
3. Viscosity $\eta = (\frac{\rho X t_l}{\rho_w X t_w})\eta_w$ … N.sec/m^2
4. Adiabatic Compressibility $\beta_a = \frac{1}{u^2\rho}$ …m^2/Newton
5. Intermolecular Free Length $L_f = K_j(\beta_a)^{1/2}$ …... m
6. Relaxation Time $\tau = \frac{4}{3}\eta\beta_a$ …… sec
7. Acoustical Impedance $Z = \rho u$ …. Kg/m^2 sec
8. Internal Pressure $P_i = \frac{\alpha T}{\beta_i}$ …. Newton/m^2

RESULTS AND DISCUSSION

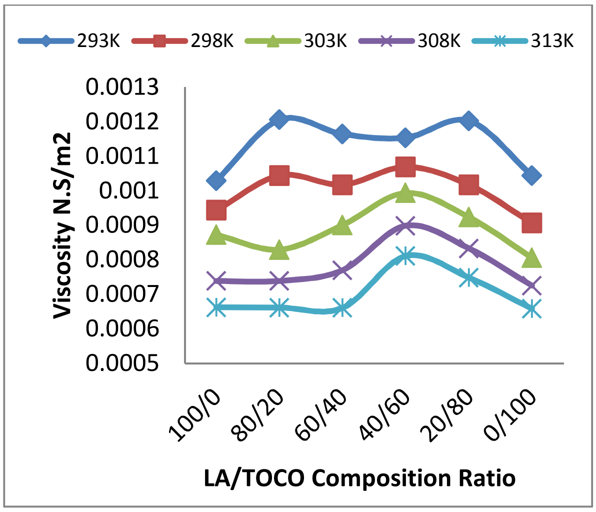
Thermo acoustical parameters are calculated using above mentioned formulae. The results are interpreted using graphs. As shown in graph [1], it is observed that ultrasonic velocity shows non-linear variation for different compositions which reflects the presence of molecular interactions. The ultrasonic velocity decreases with increase in temperature (293K to313K). The decrease in velocity may be partly due to increase in free length due to thermal expansion at higher temperature[8].The increase in molecular interactions at composition (40/60) is attributed to dipole-dipole interactions between the constituent molecules and hydrogen bonding. C=O of linoleic acid interacts with hydroxyl –OH of α-tocopherol through dipole-dipole interactions.



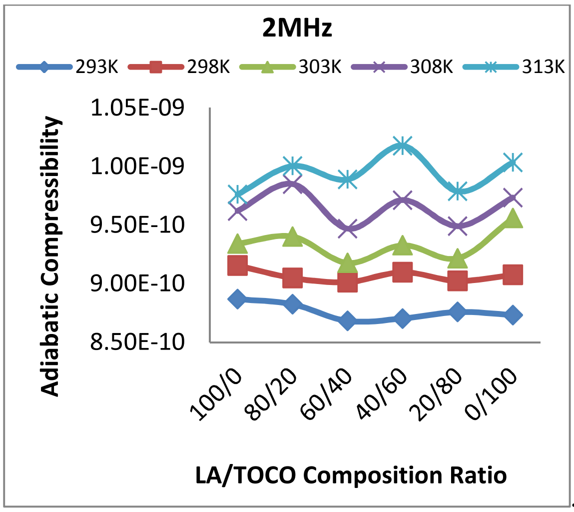
GRAPH 1



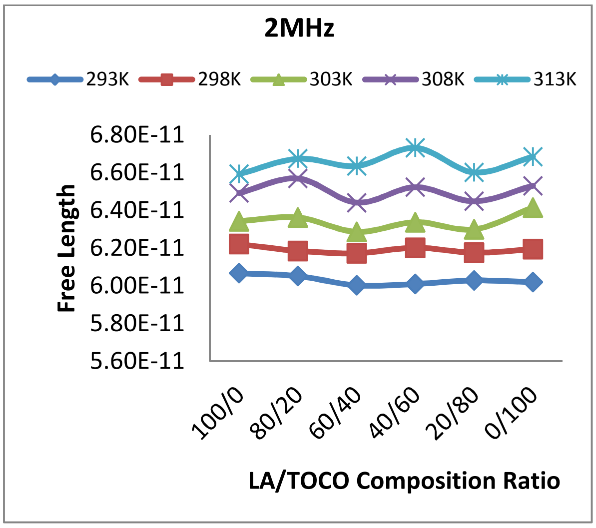
GRAPH 2



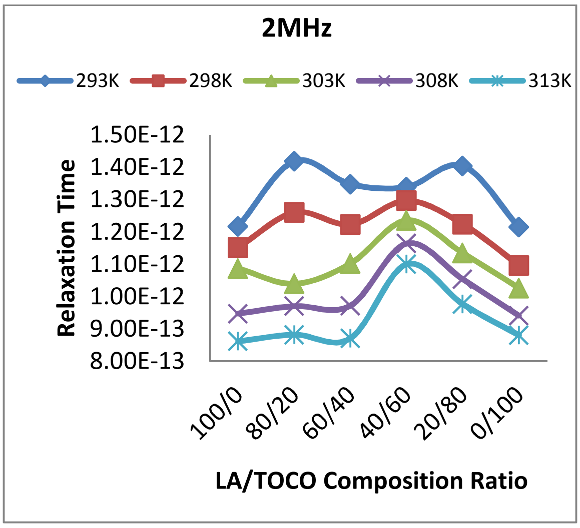
GRAPH 3



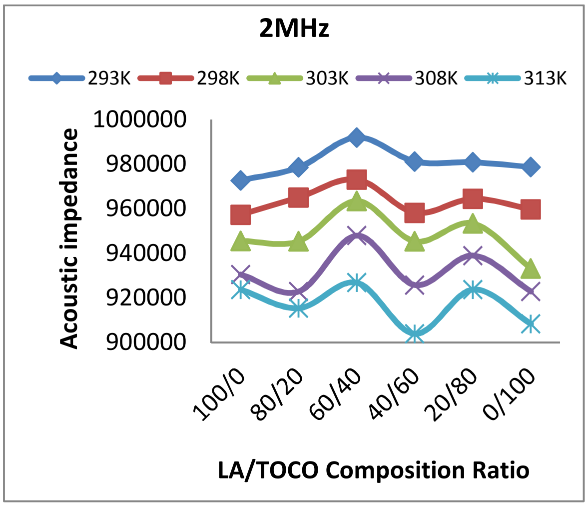
GRAPH 4



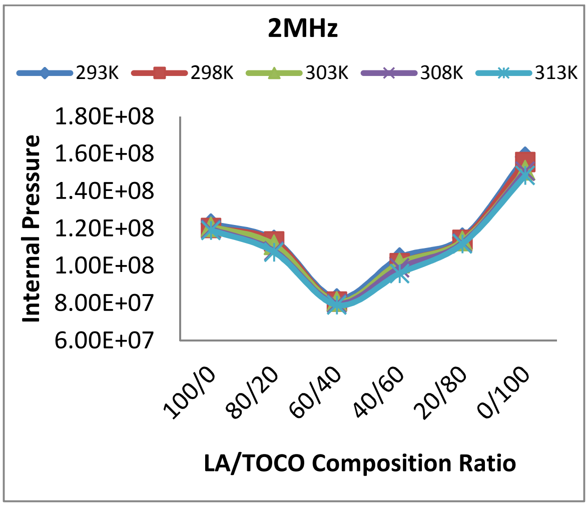
GRAPH 5



GRAPH 6



GRAPH 7



GRAPH 8

As shown in graph [2] the density decreases with increase in temperature (293K to 313K). This is because due to thermal agitations, solute molecules get more separated in solvent decreasing solute-solvent interactions. The density shows peak at (60/40) composition in LA rich region which is attributed to structure maker of solvent and strong solute solvent interactions [9].The density shows dip at (40/60) in TOCO rich region which is attributed to structure breaker of solvent due to added solute [10]. This may be due to solvent-solvent interactions bring about the bonding probably hydrogen bonding. Hence size of resultant molecule increases and density decreases.

From the graph [3], viscosity decreases with increase in temperature (293K to 313K) for different compositions indicating decrease in cohesive forces [11].Viscosity depends on molecular interactions as well as shape and size of molecules. The increase or decrease of viscosity depends on percentage of each solute in composition which in turn decides liquid structure and molecular interactions.

From the graph [4], adiabatic compressibility β_a increases with increase in temperature (293K to313K). Due to increase in temperature intramolecular bonds tend to increase due to stretching and hence compressibility increases [12]. The rise in adiabatic compressibility at composition (40/60) is due to weakening of intermolecular forces in solution and decrease in cohesive forces. The non-linear variation of adiabatic compressibility for different compositions shows molecular interactions and complex formation [13].

From the graph [5], it is observed that intermolecular free length increases with increase in temperature. The decrease in free length L_f for compositions (60/40) and (20/80) is attributed to close packing of molecules and that solute dissolves in solvent. The solute that dissolves in solvent experiences some pressure from solvent molecules [14, 15].The increase in free length L_f for compositions (80/20) and (40/60) indicates looser packing of molecules and that intermolecular cohesion is weak leading to weak molecular association [12].

From the graph [6], it is clear that relaxation time τ which depends on viscosity and adiabatic compressibility shows almost same behaviour as viscosity. With increase in viscosity the strength of intermolecular forces increases and hence relaxation time increases. Due to decrease in viscosity the strength of intermolecular forces decreases hence relaxation time also decreases.

From the graph [7], it is observed that acoustic impedance shows almost same behaviour as density with peak at (60/40) composition and dip at (40/60) composition and again slight rise at (20/80) composition. Due to increase in density at same composition intermolecular distance decreases resulting in increased dipole-dipole interactions between solute-solute and dipole-induced-dipole interactions between solute and solvent hence acoustic impedance increases.

The graph [8] shows variation in internal pressure for different compositions. Internal pressure is a measure of totality of forces of attraction, repulsion and over all cohesion between the components of molecules in solution. Internal pressure is found to decrease with increase in temperature (293K to 313K). This indicates reduction of cohesive forces as the molecules move away from each other with increase in temperature [16].From the non-linearity of internal pressure solute-solvent interactions have been confirmed [17].

CONCLUSION

1. The non-linear variation in ultrasonic velocity and other thermo acoustical parameters indicates strong solute-solute and solute-solvent interactions.
2. The molecular mechanism of compositions of linoleic acid and alpha tocopherol is known by ultrasonic investigation. Both materials are antioxidants. This data helps to improve medicine quality in drug industry.

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