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Ultrasonic Studies of Molecular Interaction Of Alcohols With Non-Polar Solvents

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Abstract

In the carbon tetrachloride / benzene method, dimethylketone measured ultrasound velocity, density and viscosity at 301 K of alcohol mixtures (pentanol, hexanol, heptanol, octanol and decanol).The following acoustical parameter was assessed from the measured values. The potential of adiabatic compression, acoustic impedance, relaxation time, relative intermolecular interlinkage with free length, free volume, available volume, constant Wadas and Rao's, Linard-John. In liquid mixtures, the essence of intermolecular interaction was dependent on the variance of the acoustic parameter.The interaction of non-polar molecules is decreasing as the length of the alcohol chains increases. Effects of molecular interactions, including dipole-dipole interaction through hydrogen bonds between solvents and 1-alkanols, were studied and interpreted. In addition, the experimental ultrasound speeds for all these binary systems are compared to the theoretical ultrasound speed

Keywords:
Ultrasonic velocity, density, binary mixtures, interaction dipole-dipole, molecular interaction, bonding hydrogen, non-polar solvents.

Introduction

An ultrasonic measurement gives an idea of the kind and nature of molecule aggregations that are present through molecular interactions in a multi-component system. Extended applications for characterising aspects of physical chemistry such as the nature of molecular interactions in pure liquids and liquor mixtures are found in ultrasonic methods.The study of the solution properties of both polar and non-polar liquid mixtures is found in applications in industrial and technological processes. The majority of the work on binary mélanges is channelled to the measurement of thermodynamic parameters such as adiabatic compression, free length, etc and their excess values to explain the molecular interactions between the binary components.In addition, such concentration studies help gain insights in the structure and bonding of the corresponding molecular complexes and molecular processes. The ultrasonic technique is used to study the properties and structures of liquids, the existence and strength of molecular interactions among fluid components Krishnamurthi etal.An study into intermolecular interaction plays a significant role in the molecular sciences; in the chemical, textile, pharmaceutical and nuclear industries there have been broad applications for liquid, liquid mixtures and solutions. The IR, Raman and dielectrical properties are also used to analyse molecular interactions. The molecular interactions for fluid alcohol mixtures with ketone have been studied at 303.15K by measuring ultra-sonic

velocity and density and expected potential interplay between different molecules.The present work deals with the ternary mixture of n-Alcohol in non-polar solvents such as carbon tetrachloride and 301K benzene (pentanol, hexanol, heptanol, octanol, decanol). The exact molecular interactions have been established between the multicomponent systems.

Methodology:

All the chemicals used in present work were analytical reagent (AR) grade (99.9% pure) and were supplied by SD fine chemicals Ltd India. The liquids were thoroughly distilled to remove dissolved impurities using standard chemical procedures. The purity of the samples was checked by the density measurements and the results were compared with the literature values. Ultrasonic velocities were measured with ultrasonic interferometer (model F80) supplied by Mittal enterprises, New Delhi, operating at a frequency of 2 MHz. It has an accuracy of ±0.1%. Viscosities of pure compounds and their mixtures were determined using Ostwald's viscometer with an accuracy of ±0.002%, calibrated with double distilled water. The densities of pure compounds and their solutions were measured accurately using 10 ml specific gravity bottles in Dhona electric balance precisely and the accuracy in weighing is ±0.1 mg. Acoustic parameters such as adiabatic compressibility (β), acoustic impedance (Z),free length (Lf), and free volume (Vf) were determined using the following relations.

Adiabatic compressibility (β)

Adiabatic compressibility were calculated from the speed of sound (u) and the density of the medium (ρ) using Newton and Laplace equation as-

$$\beta = \frac{1}{U^2 \rho}$$

Free volume (Vf)

Free volume obtained from the ultrasonic velocity (u) and the viscosity (η) of the liquid as-

$$V_f = \left(\frac{M_{eff} U}{K\eta} \right)^{3/2}$$

Relaxation time (τ)

Relaxation time calculated from the adiabatic compressibility and viscosity using the relation-

$$\tau = \frac{4}{3} \eta\beta$$

Intermolecular free length (Lf)

Estimation of intermolecular free length in liquids and in liquid mixtures has been a subject of considerable interest and semi-empirical relation to achieve the concept of intermolecular free length in order to explain the ultrasonic velocity in liquids as-

$$L_f = K_T \sqrt{\beta}.$$

Acoustic impedance (Z)

The acoustic impedance is the product of the velocity of ultrasound in a medium and its density and can be calculated by the relation is-

$$Z = U\rho$$

Relative association

Relative association can be calculated from the relation-

$$R_a = \left(\frac{\rho}{\rho_o}\right)\left(\frac{u_o}{u}\right)^{1/3}$$

ρ and ρ0 are the densities of the pure liquid and liquid mixture. u and uo are the ultrasonic velocity of pure liquid and liquid mixtures.

Available Volume and molar volume

The available volume is a direct measure of compactness and the strength of attraction between the molecules of a liquid or a mixture. It can be calculated from Schiff's relation as-

$$V_a = V\left[1-\left(\frac{u}{u_\infty}\right)\right] \quad \text{and molar volume} \quad V_m = \frac{m}{\rho}$$

Rao's constant

Rao's noted that the ratio of temperature coefficient of sound velocity u to the expansion coefficient V is virtually same for all but it is not associated with organic liquids. According to the Rao-

$$R = u^{1/3} V$$

Wada's constant

In the study of sound velocity in liquids, another constant has been suggested by Wada. According to Wada's constant –

$$W = \frac{m_{eff}}{\rho}\beta^{-1/7}$$

Lenard Jones Potential

The Lenard Jones potential is given by-

$$LJP = \frac{6v_m}{V_a}$$

Where, Vm represents the molar volume and Va represents the available volume.

Result and Discussion:

The binary mixture systems taken up for the present study are: 1- Pentanol + toluene, benzene, carbon tetrachloride, dioxane and 1-hexanol+ toluene, benzene, carbontetra chloride, dioxane and 1-heptanol + toluene, benzene, carbon tetrachloride, dioxane). The experimentally determined values of velocity, density and along with the calculated values of free volume (V_f), adiabatic compressibility (β), free length (L_f), acoustic impedance (Z) for all the systems at 301 K are reported in Table 1.

Table1.Experimentalvaluesofultrasonicvelocityanddensityofpureliquids(at301K)usedasacomponentofbinarymixtures reported in this work

Liquids	Ultrasonic velocity(m/s)	Density(Kg/ m^3)
1-Pentanol	1256	814
1-Hexanol	1288	820
1-Heptanol	1207	818
Benzene	1294	874
Toluene	1282	855
Carbontetra chloride	893	1512
Dioxane	1305	1011

In all the three binary systems, the ultrasonic velocity increases with increasing concentration of alcohols. The variation of ultrasonic velocity in a solution depends upon the increase or decrease of intermolecular free length after mixing the components.

Conclusion:

Generally, solute-solvent association arise due to slightly polar solute and polar nature of the solvent. The natures of intermolecular interaction in the liquid mixtures have been explained on the basis of the variation of acoustical parameter. An analysis of these values suggests the presence of strong intermolecular interaction in all the binary mixtures which may be due to hydrogen bond, dipole-dipole, hyperconjugation and charge transfer. It is found that the intermolecular interaction is very strong in alcohol + non-polar solvents and this strong interaction may be attributed to the fact that the interaction due to negative inductive effect dominates over the resonance effect in the mixture.

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