SUMMARY OF RESEARCH PROJECT.

UGC Reference No. : File No:47-691/08/(WRO)

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PROJECT TITLE: ULTRASONIC STUDY OF BINARY AND TERNARY LIQUID MIXTURES CONTAINING POLAR AND NON POLAR LIQUIDS AT DIFFERENT TEMPERATURE.

Now a day's ultrasonic study is a subject of extensive research and usefulness in the field of biology, biochemistry, dentistry engineering, geography, geology, medicine, Polymers, industry etc. It has been applied to process monitoring and material characterization. Ultrasonic velocity together with density and viscosity data fields to get the information about interactions between ions, dipoles H-bonding, multi-polar and dispersion process. Ultrasonic studies help to understand the molecular interaction and structure formation in binary as well as ternary liquid mixtures.

In this project, the molecular interaction, dipole-dipole interaction, collision factors and hydrogen bond forces in binary and ternary liquid systems containing polar and non polar liquids at different temperature. The binary liquids systems under investigation are,

1) Acetone in butanol
2) Picoline in ethanol
3) Thiophene in ethanol

The liquids which were use are BDH analar grade and distilled twice in laboratory. The mixtures of middle fraction will be prepared immediately before use in appropriate volume at room temperature. The ultrasonic velocity will be measured by pulse echo overlap method. The density of pure liquids and their mixtures will be measured by the hydrostatic plunger method. A cell will be designed be consists of double walled cylindrical glass vessel. The fast rise dual trace oscilloscope is used to observe the time interval and intensities of ultrasonic pulse. Thermostat is used to obtain good stability of temperature. It is used for circulating the water at a constant temperature around the measuring cell in the range 20°C to 45°C .In the binary liquid system under investigation, the variation of ultrasonic velocity (u) and excess adiabatic compressibility (β_a) indicate existence of molecular interaction between solvent and solute. The excess adiabatic compressibility B_a^E is positive over whole concentration range and it becomes minimum at a concentration (0.5) of α-picoline in ethanol at observed temperatures. This indicates that the intermolecular interaction at this optimum at this concentration and it may leads to formation weak hydrogen bonded complex in binary liquid mixture. The same effects are also observed in excess volume (V^E) and excess viscosity (η^E). The Grunberg and Nissan parameter (*d*) which indicate the extent of molecular interaction[6] in the liquid mixture also shows same variations over the whole concentration range. This conclusion is further supported by thermodynamic studies on a similar system by IR and NMR.It is observed that beyond this optimum concentration, addition of solute (α-picoline) in a solvent (ethanol) tries to break this weak complex structure and tends towards the values of pure components. The presence of hydroxyl group and shortness of chain of the carbon in ethanol is responsible to participate in hydrogen bonding leads to the association with the molecules of α-picoline. It is evident that in the case of α-picoline, the normal inductive effect of methyl group has interaction with ethanol is also observed.

The theoretical computed values of ultrasonic velocities by using Nomatos empirical formula, Vandeel and Vangeel expression based on Richardson's assumptions ,Junjie method ,Impedance dependence relation and collision factory theory with experimental values are computed over whole concentration of a-picoline in ethanol, Acetone in butanol and Thiophene in ethanol at 301.15K. The molecular interaction parameter (MIP) and percentage deviation of ultrasonic velocity is also computed and discuss in terms of molecular interactions in these binary systems. The validity of these theories is checked by applying Chi-square test and average percentage error.

The variation in theoretical values of ultrasonic velocities over whole concentration range is shown in the form of variation on graphs. Similarly variation in percentage deviation is for the Nomats relation shows the

negative deviation over whole concentration and present in the range – 2.7013 to – 5.7687. According to Vandeel and vangeels ideal mixing relation the deviation is positive and present in the range 1.6701 to 8.5097.Junjies relation , collision factor theory and Impedance dependence relation shows the deviation in the range – 1.5988 to – 4.1486, -2.1904 to +0.5940 and – 4.7058 to –2.0705 respectively. These binary systems indicate that the percentage error is minimum for CFT hence it predicts the values of ultrasonic velocities close to experimental values for binary mixture containing a- picoline in ethanol. The theory proposes by Vandeel and vangeels using ideal mixing relation shows the maximum deviation in theoretical values from experimental values.

The acoustic data of ultrasonic velocity (u), density (ρ), viscosity (η) and Related thermodynamic parameters with their excess values of α- picoline inethanol over the whole concentration range may suggest the existence of a strongmolecular interaction in binary liquid mixture. The negative values of some thermo-acoustic parameters like excess compressibility indicate a strong intermolecular interaction in the constitute molecules due to presence of hydroxyl group of binary liquid mixture and it may leads to the formation of weak complex in the liquid mixture at particular concentration. In this work CFT, Nomatos, Vandeel and vangeels ideal mixing, Jungies and Impedance dependence relations are used to calculate ultrasonic velocities in the binary mixture containing a – picoline in ethanol at 302.15K.From these theoretically calculated values it is conclude that the collision factory theory proposed by Shaft and Nutsch-Kuhnkies is found to best suited with experimental values having minimum percentage error.

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