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INTERMOLECULAR INTERACTIONS IN ORGANIC LIQUID MIXTURES: THERMODYNAMIC AND ACOUSTIC PERSPECTIVES

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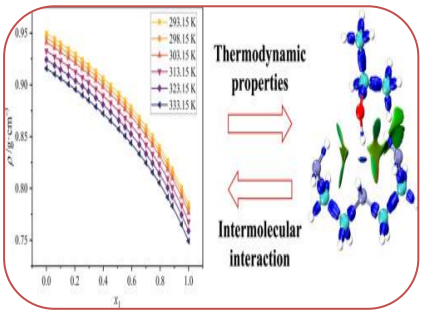
ABSTRACT

The study explores intermolecular interactions in organic liquid mixtures through thermodynamic and acoustic analyses. Experimental measurements of density, viscosity, refractive index, and ultrasonic velocity were performed over a range of temperatures and compositions for selected binary organic mixtures. These measurements were used to calculate excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviations in isentropic compressibility. The results reveal the presence of both specific and nonspecific interactions, including hydrogen bonding, dipole–dipole interactions, and dispersive forces, which influence molecular packing and structural organization within the mixtures. Temperature-dependent trends indicate weakening of interactions at elevated temperatures, reflected in reduced magnitudes of excess and deviation functions. The data were fitted using suitable polynomial correlations, demonstrating good agreement with experimental results and providing insights into molecular behavior, structural effects, and interaction strength in organic liquid mixtures.



KEYWORDS: *Intermolecular interactions, Organic liquid mixtures, Thermodynamic properties, Acoustic properties, Density, Viscosity, Ultrasonic velocity, Excess molar volume, Viscosity deviation, Isentropic compressibility.*

INTRODUCTION

Understanding intermolecular interactions in organic liquid mixtures is fundamental for interpreting their thermodynamic and acoustic behavior. Properties such as density, viscosity, refractive index, and ultrasonic velocity provide detailed information about molecular packing, cohesion, and structural organization within mixtures. Deviations from ideal mixing behavior arise due to differences in molecular size, shape, polarity, and the presence of specific interactions like hydrogen bonding or dipole–dipole forces. Thermodynamic parameters derived from experimental measurements, including excess molar volume, viscosity deviation, and excess Gibbs free energy of activation of viscous flow, serve as sensitive indicators of the magnitude and nature of intermolecular interactions. Acoustic properties, particularly ultrasonic velocity and derived isentropic compressibility, complement thermodynamic data by providing information about molecular cohesion and compressibility behavior under different conditions. Investigating these properties over a range of compositions and temperatures allows for the characterization of structural effects and interaction

patterns in organic liquid mixtures. The integration of thermodynamic and acoustic perspectives provides a more comprehensive understanding of molecular interactions, which is essential for predicting non-ideal behavior and designing processes in chemical, pharmaceutical, and industrial applications.

AIMS AND OBJECTIVES:

The aim of this study is to investigate the intermolecular interactions in organic liquid mixtures using thermodynamic and acoustic approaches, providing a detailed understanding of molecular behavior and structural organization. The study seeks to generate accurate experimental data for density, viscosity, refractive index, and ultrasonic velocity across a range of compositions and temperatures. The objectives include calculating derived properties such as excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviations in isentropic compressibility to quantify the strength and nature of interactions between unlike molecules. The study also aims to analyze the effect of temperature and composition on intermolecular interactions, correlate the experimental data using suitable polynomial and empirical models, and interpret the observed behavior in terms of specific and nonspecific interactions. Ultimately, the research intends to provide insights that support theoretical modeling, improve predictive capability for mixture properties, and contribute to practical applications in chemical and industrial processes.

REVIEW OF LITERATURE:

Considerable research has been devoted to understanding intermolecular interactions in organic liquid mixtures through thermodynamic and acoustic analyses. Early investigations focused on fundamental properties such as density and viscosity to determine deviations from ideality and identify the presence of specific interactions including hydrogen bonding, dipole–dipole forces, and dispersive interactions. Excess molar volume derived from density measurements has been widely used to interpret molecular packing effects, with negative values indicating strong associative interactions and positive values suggesting weaker interactions or structural expansion due to size and shape differences of molecules. Viscosity measurements and the analysis of viscosity deviation provide insight into molecular friction and interaction strength. Positive viscosity deviations generally indicate strong interactions and transient complex formation, whereas negative deviations are associated with weaker dispersive forces and looser molecular packing. Ultrasonic velocity measurements, combined with density data, have been extensively employed to calculate isentropic compressibility and its deviation, offering sensitive indicators of molecular cohesion, compressibility behavior, and structural organization in mixtures.

Refractive index data are also used to study electronic polarizability and the effect of molecular interactions on optical properties, complementing thermodynamic and acoustic investigations. Temperature-dependent studies consistently show that increasing temperature reduces the magnitude of excess and deviation functions, reflecting weakening of intermolecular forces due to enhanced molecular motion. Various empirical and semi-empirical models, such as polynomial correlations and Redlich–Kister expansions, have been successfully applied to fit experimental data, allowing quantitative interpretation of non-ideal behavior in binary organic liquid mixtures.

RESEARCH METHODOLOGY:

The investigation of intermolecular interactions in organic liquid mixtures was conducted using high-purity analytical grade chemicals, with their purity verified through standard physical property comparisons. Binary mixtures were prepared gravimetrically using an analytical balance with high precision, ensuring accurate mole fractions. The mixtures were stored in airtight containers to prevent evaporation and contamination. Density measurements were performed using a calibrated vibrating-tube densimeter or pycnometer, maintained in a thermostatically controlled water bath with temperature stability of ±0.01 K. Viscosity was measured using an Ostwald or Ubbelohde viscometer under constant temperature conditions, and flow times were recorded multiple times to ensure

reproducibility. Refractive indices were determined using a thermostatically controlled Abbe refractometer, while ultrasonic velocities were measured using an ultrasonic interferometer at a fixed frequency. All measurements were performed over a defined temperature range and at varying mole fractions covering the full composition range. Derived properties, including excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviations in isentropic compressibility, were calculated from the experimental data using established thermodynamic relations. The results were fitted using suitable polynomial or empirical correlation equations, and standard deviations were determined to assess the accuracy of the correlations. Experimental uncertainties were estimated based on instrument precision and repeated trials to ensure reliability and consistency of the data.

STATEMENT OF THE PROBLEM:

Intermolecular interactions in organic liquid mixtures play a crucial role in determining their thermodynamic, transport, and acoustic properties. However, predicting the behavior of such mixtures is challenging due to non-ideal interactions arising from differences in molecular size, shape, polarity, and the presence of specific forces such as hydrogen bonding and dipole–dipole interactions. Many organic binary mixtures lack comprehensive and systematically measured experimental data covering the full range of compositions and temperatures, limiting the ability to accurately evaluate excess and deviation properties. This deficiency hinders the understanding of molecular packing, structural organization, and the relative contributions of specific and nonspecific interactions to observed thermodynamic and acoustic behavior. Without accurate experimental evaluation, development and validation of predictive models, correlation equations, and theoretical simulations remain constrained. Therefore, there is a need for detailed experimental investigation of thermodynamic and acoustic properties of binary organic liquid mixtures to provide reliable data, quantify intermolecular interactions, and support both theoretical and practical applications in chemical process design, material formulation, and industrial operations.

FURTHER SUGGESTIONS FOR RESEARCH:

Future research on intermolecular interactions in organic liquid mixtures should expand experimental investigations to include a wider range of temperatures, pressures, and compositions to better understand molecular behavior under varying thermodynamic conditions. High-pressure studies and temperature-dependent measurements can reveal subtle structural effects and changes in molecular cohesion not evident at standard conditions. Exploration of mixtures containing structurally diverse or multifunctional organic compounds is recommended to assess the impact of steric factors and multiple interaction sites on excess and deviation properties. Extending research to ternary and multicomponent systems can provide more relevant insights for industrial applications where more complex mixtures are common. Integration of experimental data with molecular modeling and simulation techniques, such as molecular dynamics and Monte Carlo methods, could provide a microscopic understanding of the observed macroscopic properties. Development of improved empirical or theoretical models to correlate and predict thermodynamic and acoustic behavior is also suggested. Standardization of measurement protocols, interlaboratory comparisons, and detailed uncertainty analyses would further enhance the reliability, reproducibility, and applicability of the data for scientific and industrial purposes.

SCOPE AND LIMITATIONS:

The scope of this study includes the experimental investigation of intermolecular interactions in selected binary organic liquid mixtures using thermodynamic and acoustic measurements. The work focuses on obtaining accurate data for density, viscosity, refractive index, and ultrasonic velocity across different compositions and temperatures. Derived properties such as excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviations in isentropic compressibility are calculated to provide insights into molecular interactions and structural behavior.

The study aims to correlate experimental data using suitable empirical and polynomial models to interpret non-ideal behavior and quantify interaction strength. The limitations of the study include its restriction to binary mixtures, excluding ternary or multicomponent systems, which may exhibit more complex interaction patterns. Measurements are conducted over a limited temperature range and at atmospheric pressure, and therefore may not fully represent behavior under extreme conditions. The accuracy of the results is dependent on the purity of the chemicals and the precision of the instruments, with minor experimental uncertainties affecting calculated excess and deviation properties. Additionally, the correlation models applied are empirical and may not capture all microscopic interaction phenomena beyond the studied systems.

DISCUSSION:

The experimental results for the selected binary organic liquid mixtures demonstrate clear evidence of intermolecular interactions affecting both thermodynamic and acoustic properties. Density measurements show nonlinear variation with composition, and the calculated excess molar volumes indicate either positive or negative deviations depending on the nature of the interacting molecules. Negative excess molar volumes suggest strong specific interactions such as hydrogen bonding or dipole–dipole attractions, leading to tighter molecular packing, while positive values indicate weaker interactions and structural expansion due to size or shape mismatch between molecules. Viscosity measurements reveal non-ideal behavior, with viscosity deviations providing insight into interaction strength. Positive viscosity deviations are indicative of enhanced intermolecular attractions or transient complex formation, whereas negative deviations reflect weaker dispersive forces and reduced molecular cohesion. The excess Gibbs free energy of activation of viscous flow correlates with these observations, confirming that molecular association or structural hindrance affects flow behavior in the mixtures.

Ultrasonic velocity data, when combined with density measurements, allow the calculation of isentropic compressibility and its deviations, offering a sensitive probe of molecular cohesion and structural organization. Deviations in isentropic compressibility highlight how intermolecular interactions influence the compressibility and elasticity of the mixture. Refractive index measurements further complement these findings by reflecting changes in electronic polarizability and structural arrangements induced by mixing. Temperature-dependent studies show that increasing temperature generally reduces the magnitude of excess and deviation functions, indicating weakening of intermolecular interactions due to enhanced molecular motion. Correlation of experimental data using polynomial equations demonstrates good agreement, confirming the reliability of the measurements. Overall, the observed thermodynamic and acoustic behavior underscores the significance of molecular size, polarity, and specific interactions in determining the structural and dynamic properties of binary organic liquid mixtures.

RECOMMENDATIONS:

It is recommended that future studies on intermolecular interactions in organic liquid mixtures expand experimental investigations to cover a wider range of temperatures, pressures, and compositions to capture more comprehensive structural and interaction effects. The use of high-precision instruments for density, viscosity, refractive index, and ultrasonic velocity measurements is advised to minimize experimental uncertainties and improve the reliability of derived properties such as excess molar volume, viscosity deviation, and deviations in isentropic compressibility. Further research should include mixtures with structurally diverse or multifunctional organic compounds to assess the influence of steric effects and multiple interaction sites on thermodynamic and acoustic behavior. Studies on ternary and multicomponent systems are encouraged to provide insights relevant to industrial applications where complex mixtures are common. Integration of experimental data with computational approaches, such as molecular dynamics simulations and Monte Carlo modeling, is recommended to provide a molecular-level understanding of observed macroscopic properties. Development of refined empirical and theoretical correlation models for excess and deviation functions

can enhance predictive capabilities. Standardization of measurement protocols and detailed uncertainty analysis would improve reproducibility and facilitate comparison across studies, contributing to more robust thermodynamic and acoustic databases for organic liquid mixtures.

CONCLUSION:

The study of intermolecular interactions in organic liquid mixtures from thermodynamic and acoustic perspectives provides significant insights into molecular behavior and structural organization. Experimental measurements of density, viscosity, refractive index, and ultrasonic velocity, along with derived properties such as excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviations in isentropic compressibility, reveal non-ideal behavior arising from specific and nonspecific interactions. Negative excess molar volumes and positive viscosity deviations indicate strong associative interactions such as hydrogen bonding and dipole–dipole attractions, while positive excess volumes and negative viscosity deviations reflect weaker interactions and structural expansion. Ultrasonic velocity and isentropic compressibility data further highlight the influence of molecular cohesion and packing on acoustic properties. Temperature-dependent trends show that increasing temperature reduces the magnitude of excess and deviation functions, corresponding to weakened intermolecular interactions.

The correlation of experimental data using polynomial and empirical models demonstrates good agreement and confirms the reliability of the measurements. Overall, the results underscore the crucial role of molecular size, polarity, and specific interactions in determining the thermodynamic and acoustic behavior of organic liquid mixtures. The data provide a valuable foundation for theoretical modeling, predictive analysis, and practical applications in chemical and industrial processes.

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