



## THERMODYNAMIC AND TRANSPORT PROPERTIES OF BINARY ORGANIC LIQUID MIXTURES

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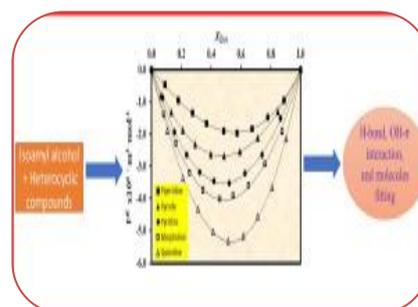
### ABSTRACT

The thermodynamic and transport properties of binary organic liquid mixtures were investigated over a range of temperatures and compositions. Experimental densities, viscosities, refractive indices, and ultrasonic velocities were measured and used to evaluate excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviation in isentropic compressibility. The results indicate the presence of specific and nonspecific intermolecular interactions depending on composition and temperature. The data were correlated using suitable polynomial equations, and standard deviations were calculated to assess the accuracy of fitting. The observed variations in excess and deviation functions reveal structural effects and molecular interactions within the mixtures. Several empirical and semi-empirical models, including polynomial, Redlich-Kister, and other correlation equations, have been applied to fit experimental excess and deviation functions, facilitating quantitative description of non-ideal behavior. Literature reports emphasize the effect of temperature on excess properties, where increased thermal motion tends to diminish intermolecular interactions.

**KEYWORDS:** Thermodynamic properties, Transport properties, Binary organic liquid mixtures, Density, Viscosity, Excess molar volume, Viscosity deviation, Intermolecular interactions, Isentropic compressibility.

### INTRODUCTION

The study of thermodynamic and transport properties of binary organic liquid mixtures provides essential information for understanding molecular interactions and structural behavior in liquid systems. Properties such as density, viscosity, refractive index, ultrasonic velocity, and related excess and deviation functions are fundamental for the design and optimization of chemical processes including distillation, extraction, and heat transfer operations. These properties offer insight into intermolecular forces such as hydrogen bonding, dipole-dipole interactions, and dispersion forces that govern the non-ideal behavior of liquid mixtures. Binary organic liquid mixtures often exhibit deviations from ideality due to differences in molecular size, shape, and polarity of the constituent components. Evaluation of excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviation in isentropic compressibility enables quantitative assessment of the strength and nature of interactions between unlike molecules. Positive or negative deviations in these parameters reflect structural effects, packing efficiency, and specific association phenomena occurring in the mixture. Accurate experimental determination of



thermodynamic and transport properties over a range of temperatures and compositions is crucial for developing reliable predictive models and correlating equations. Such data contribute significantly to thermodynamic databases and support the validation of theoretical models describing liquid-phase behavior.

### **AIMS AND OBJECTIVES:**

The aim of this study is to investigate the thermodynamic and transport properties of binary organic liquid mixtures over a range of temperatures and compositions in order to understand the nature and strength of intermolecular interactions present in the system. The work seeks to obtain accurate experimental data for density, viscosity, refractive index, and ultrasonic velocity and to evaluate derived excess and deviation properties such as excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviation in isentropic compressibility. The objectives include analyzing the non-ideal behavior of the mixtures through interpretation of excess functions, correlating the experimental results using suitable mathematical models, determining the effect of temperature on molecular interactions and structural arrangement, and assessing the applicability of theoretical and empirical equations in representing the observed data. The study also aims to contribute reliable thermodynamic and transport property data to support process design, modeling, and industrial applications involving organic liquid mixtures.

### **REVIEW OF LITERATURE:**

Extensive research has been conducted on the thermodynamic and transport properties of binary organic liquid mixtures to elucidate the influences of molecular interactions and structural effects on liquid-phase behavior. Early studies focused on fundamental properties such as density and viscosity to interpret deviations from ideal mixing behavior and to identify the presence of specific interactions such as hydrogen bonding, dipole–dipole attractions, and van der Waals forces. Researchers have reported that excess molar volume, often derived from density measurements, can exhibit positive or negative values depending on the relative size and polarity of the constituent molecules, reflecting changes in packing efficiency and free volume within the mixture. Viscosity measurements and the evaluation of viscosity deviation have been widely used to characterize the strength of molecular interactions, with negative viscosity deviations frequently attributed to the dominance of weak dispersive forces and positive deviations indicating strong associative interactions. Refractive index data have been employed to calculate excess refractive index and related optical properties, providing further insights into electronic polarizability and interaction-induced structural changes. Ultrasonic velocity measurements, combined with density data, have enabled the determination of isentropic compressibility and deviation in isentropic compressibility, which are sensitive indicators of molecular cohesion and compressional behavior in liquid mixtures.

### **RESEARCH METHODOLOGY:**

The experimental investigation of thermodynamic and transport properties of binary organic liquid mixtures was carried out using high-purity analytical grade chemicals without further purification. The purity of each component was verified by comparing measured densities and viscosities with standard literature values. Binary mixtures were prepared gravimetrically using an analytical balance with high precision, and the uncertainty in mole fraction was minimized by careful mass measurements. The prepared mixtures were stored in airtight containers to prevent evaporation and contamination. Density measurements were performed using a calibrated pycnometer or vibrating-tube densimeter maintained in a thermostatically controlled water bath with temperature stability within  $\pm 0.01$  K. Viscosity measurements were carried out using an Ostwald or Ubbelohde viscometer, also immersed in a constant-temperature bath to ensure thermal equilibrium before each reading. Flow times were recorded using a digital stopwatch, and multiple measurements were taken to ensure reproducibility. Refractive index measurements were conducted with a thermostatically controlled Abbe refractometer, while ultrasonic velocity was determined using an ultrasonic interferometer.

operating at a fixed frequency. All measurements were performed over a selected temperature range and at different mole fractions covering the entire composition range. Derived thermodynamic and transport properties such as excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviation in isentropic compressibility were calculated from the experimental data using standard thermodynamic relations. The excess and deviation functions were correlated using suitable polynomial equations, and standard deviations were evaluated to assess the accuracy of the fitting.

#### **STATEMENT OF THE PROBLEM:**

Accurate knowledge of thermodynamic and transport properties of binary organic liquid mixtures is essential for understanding molecular interactions and for the reliable design of chemical and industrial processes. However, many organic liquid systems exhibit non-ideal behavior due to differences in molecular size, shape, and polarity, leading to deviations from ideal mixing laws. In several cases, available experimental data are limited, inconsistent, or unavailable over a wide range of temperatures and compositions, creating difficulties in predicting mixture behavior with precision. The lack of comprehensive and systematically measured data on properties such as density, viscosity, refractive index, ultrasonic velocity, and their corresponding excess and deviation functions restricts the development and validation of theoretical models and correlation equations. Without accurate experimental evaluation, it becomes challenging to interpret the nature and strength of intermolecular interactions and to apply the data confidently in process design, simulation, and optimization. Therefore, there is a need for detailed experimental investigation and analysis of thermodynamic and transport properties of selected binary organic liquid mixtures to generate reliable data, assess non-ideal behavior, and contribute to a better understanding of molecular interactions in liquid systems.

#### **FURTHER SUGGESTIONS FOR RESEARCH:**

Further research on thermodynamic and transport properties of binary organic liquid mixtures may focus on extending experimental investigations to wider temperature and pressure ranges in order to obtain a more comprehensive understanding of molecular interactions under varying thermodynamic conditions. Studies involving high-pressure measurements would provide valuable insight into structural effects and compressibility behavior that are not evident at atmospheric pressure. Future work may also include the examination of mixtures containing structurally complex or multifunctional organic compounds to explore the influence of steric effects and multiple interaction sites on excess and deviation properties. Investigations of ternary and multicomponent systems could enhance the applicability of experimental data to real industrial formulations where more than two components are present. The integration of experimental data with advanced theoretical models and molecular simulation techniques such as molecular dynamics and Monte Carlo methods could further clarify the microscopic origin of observed macroscopic properties. Development and validation of improved predictive models and equations of state based on extensive datasets would strengthen the reliability of property estimation methods. Additionally, systematic uncertainty analysis and interlaboratory comparisons are recommended to enhance data accuracy and reproducibility, thereby contributing to robust thermodynamic databases and improved process design methodologies.

#### **SCOPE AND LIMITATIONS:**

The scope of the present study encompasses the experimental determination and analysis of thermodynamic and transport properties of selected binary organic liquid mixtures over a defined range of temperatures and compositions. The investigation includes the measurement of fundamental properties such as density, viscosity, refractive index, and ultrasonic velocity, along with the evaluation of derived excess and deviation functions including excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviation in isentropic compressibility. The study aims to interpret the nature of intermolecular interactions and structural effects responsible for non-ideal behavior in liquid mixtures and to correlate the experimental data using suitable mathematical

models. However, the study is limited to binary systems and does not extend to ternary or multicomponent mixtures, which may exhibit more complex interaction patterns. The experimental work is conducted within a specific temperature range and at atmospheric pressure, and therefore the results may not represent behavior under extreme conditions such as high pressure or very wide temperature variations. The accuracy of the results depends on the precision of the instruments used and the purity of the chemicals, and minor experimental uncertainties may influence the calculated excess and deviation properties. Furthermore, the correlations applied are empirical in nature and may not fully describe molecular-level phenomena beyond the studied systems.

### DISCUSSION:

The measured thermodynamic and transport properties of the binary organic liquid mixtures exhibit systematic variations with composition and temperature, indicating significant deviations from ideal behavior. The density data show nonlinear dependence on mole fraction, and the calculated excess molar volumes reveal either positive or negative values depending on the nature of the interacting components. Negative excess molar volumes suggest strong specific interactions such as hydrogen bonding or dipole-dipole attractions leading to closer packing of unlike molecules, whereas positive values indicate weaker interactions and structural expansion due to differences in molecular size and shape. Viscosity values increase or decrease with composition in a non-linear manner, reflecting changes in intermolecular friction and molecular association. The viscosity deviation data provide further insight into interaction strength. Positive viscosity deviations imply enhanced intermolecular attractions and formation of transient complexes, while negative deviations indicate dominance of dispersive forces and structural loosening in the mixture. The excess Gibbs free energy of activation of viscous flow supports these interpretations, as its magnitude and sign correlate with the degree of molecular interaction and resistance to flow.

### RECOMMENDATIONS:

It is recommended that future investigations on thermodynamic and transport properties of binary organic liquid mixtures include systematic measurements over broader temperature and pressure ranges to improve the understanding of interaction mechanisms under varying thermodynamic conditions. The use of high-precision digital instruments and advanced temperature control systems is encouraged to reduce experimental uncertainties and enhance data reliability. Careful purification of chemicals and verification of component properties prior to mixture preparation are also recommended to ensure accuracy of results. Further studies should emphasize the collection of comprehensive datasets covering the entire composition range to enable more accurate evaluation of excess and deviation functions. Application of advanced correlation models and comparison with theoretical predictions are recommended to strengthen interpretation of molecular interactions. Incorporation of computational approaches such as molecular simulation techniques may provide deeper insight into microscopic structural behavior and complement experimental findings.

### CONCLUSION:

The investigation of thermodynamic and transport properties of binary organic liquid mixtures provides valuable insights into the nature and strength of intermolecular interactions and the structural behavior of liquid systems. Experimental measurements of density, viscosity, refractive index, and ultrasonic velocity, along with the evaluation of derived properties such as excess molar volume, viscosity deviation, excess Gibbs free energy of activation of viscous flow, and deviation in isentropic compressibility, reveal significant deviations from ideal behavior, indicating the presence of specific and nonspecific molecular interactions. The study demonstrates that negative excess molar volumes and positive viscosity deviations are indicative of strong associative interactions, while positive excess molar volumes and negative viscosity deviations reflect weaker interactions and structural expansion. Temperature has a consistent effect in reducing the magnitude of excess and deviation functions due to increased thermal motion and weakening of molecular interactions. Correlation of experimental data

using polynomial equations shows good agreement with observed values, confirming the reliability of the measurements and analysis. Overall, the findings emphasize the critical role of molecular size, polarity, and specific interactions in determining the thermodynamic and transport behavior of binary organic liquid mixtures. The data generated from this study can serve as a valuable reference for theoretical modeling, process design, and optimization in chemical and industrial applications.

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