

Ultrasound Velocity Analysis for Molecular Interactions in Binary Liquid Mixtures of Cumene and Propanone-2 across Variable Temperatures

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KEYWORDS

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ABSTRACT

Presented study explores molecular interactions in binary liquid mixtures of cumene and propanone-2 through the measurement of ultrasonic velocity, density, and viscosity at temperatures of 303 K, 308 K, and 313 K. The derived acoustic and thermodynamic parameters—including isentropic compressibility, intermolecular free length, molar volume, relaxation time, and Rao's constant—were systematically analyzed to elucidate interaction mechanisms at the molecular level. Additionally, excess parameters were computed to assess deviations from ideal behavior, providing deeper insights into molecular association and structural modifications induced by temperature variations. The findings reveal prominent dipole-dipole interactions between the constituent molecules, modulated by thermal effects, highlighting the complex interplay of cohesive and dispersive forces in polar liquid mixtures. This research advances the fundamental understanding of liquid-phase interactions, offering valuable implications for industrial and chemical applications, including solvent formulation, reaction dynamics, and material design.

1. Background

The study of molecular interactions in liquid mixtures is a cornerstone of physical chemistry, essential for understanding the equilibrium behavior and structural dynamics of chemical systems. Molecular interactions dictate various macroscopic properties, influencing fields such as chemical engineering, pharmaceuticals, and material science. The investigation of these interactions through ultrasonic velocity measurements provides a powerful and non-destructive means to characterize the underlying intermolecular forces governing liquid mixtures. Ultrasonic velocity and its derived acoustic and thermodynamic parameters serve as valuable tools in examining deviations from ideal behavior in liquid mixtures, which arise due to specific molecular interactions such as hydrogen bonding, dipole-dipole forces, and dispersion interactions. These deviations provide insight into molecular organization, structural modifications, and energy exchanges occurring within the mixture. Notably, previous research has underscored the importance of temperature and composition in influencing acoustic parameters in binary liquid systems. Patil and Naik (4) demonstrated the impact of temperature variations on ultrasonic properties, highlighting their critical role in determining molecular interactions. Similarly, Kolhe and Bhosale (5) reported that increasing temperature leads to a weakening of molecular interactions due to the disruption of structured molecular networks. Despite extensive studies on binary liquid mixtures, a detailed analysis of polar systems, such as cumene and propanone-2, remains relatively unexplored. Both compounds exhibit significant dipole-dipole interactions, making them ideal candidates for an in-depth investigation into their acoustic and thermodynamic behavior. Understanding the interactions

within such mixtures is crucial for applications in solvent chemistry, industrial formulations, and reaction dynamics. This study aims to fill this research gap by analyzing the acoustic and thermodynamic properties of cumene-propanone-2 mixtures across different concentrations and temperatures (303 K, 308 K, and 313 K). The derived parameters, including isentropic compressibility, intermolecular free length, and excess thermodynamic functions, are examined to elucidate the nature and extent of molecular interactions in the system. By providing a systematic evaluation of dipole-dipole interactions in polar binary mixtures, this research contributes to the broader understanding of molecular association phenomena and their implications in industrial and scientific applications.

2. Methodology

2.1 Materials

The binary liquid mixtures of cumene (isopropylbenzene) and propanone-2 (acetone) were prepared using high-purity analytical reagent-grade chemicals sourced from Loba Chemicals. The purity of the chemicals was verified by cross-referencing their boiling points and densities with standard values reported in the literature. Both components were subjected to a drying process using anhydrous calcium chloride to eliminate any residual moisture and were subsequently purified through fractional distillation to ensure high purity and reproducibility of results.

2.2 Preparation of Mixtures

The binary mixtures of cumene and propanone-2 were prepared in varying mole fractions, ranging from 0 to 1, to systematically investigate their physicochemical properties. The mixtures were prepared in pre-cleaned, airtight glass containers to prevent contamination. Homogenization was achieved using a magnetic stirrer to ensure uniform mixing, and the prepared mixtures were stored in desiccators to prevent moisture absorption and evaporation, thereby maintaining sample integrity throughout the experimental procedures.

2.3 Experimental Setup

All experimental measurements were conducted in a thermostatically controlled water bath, ensuring temperature stability with an accuracy of $\pm 0.1^\circ\text{C}$. The temperature conditions for all samples were set at 303 K, 308 K, and 313 K to examine the temperature dependence of molecular interactions in the binary mixtures. This controlled setup facilitated precise and reproducible measurements, minimizing environmental variability.

2.4 Measurement Techniques

2.4.1. Ultrasonic Velocity Measurement: Ultrasonic velocity measurements were carried out using an ultrasonic interferometer (Model F-81, Mittal Enterprises, New Delhi) operating at a fixed frequency of 2 MHz. The instrument was pre-calibrated using standard liquids, and the measurement uncertainty was maintained within $\pm 0.5\%$. These measurements provided insights into the molecular interactions and structural modifications within the binary liquid system.

2.4.2. Density Determination: The densities of the prepared mixtures were measured using a double-walled bi-capillary pycnometer. The instrument was calibrated with distilled water, and corrections were applied to account for buoyancy effects and temperature fluctuations. The

uncertainty in density measurements was limited to $\pm 0.001 \text{ g/cm}^3$, ensuring high precision in the evaluation of volumetric properties of the mixtures.

2.4.3. Viscosity Measurement: Viscosity measurements were performed using a calibrated Ubbelohde viscometer. A fixed volume of each liquid mixture was drawn into the viscometer, and the flow time was recorded using a digital stopwatch. The viscosity values were determined using the known calibration constant of the viscometer, with an error margin of $\pm 0.002 \text{ cP}$. These measurements facilitated an understanding of the rheological behavior and intermolecular forces within the binary mixtures.

2.5 Data Analysis and Interpretation

The obtained experimental data for ultrasonic velocity, density, and viscosity were analyzed to assess molecular interactions, structural modifications, and thermophysical properties of the binary mixtures. The temperature-dependent variations in these properties were systematically evaluated to establish their correlation with intermolecular forces. Regression analysis and theoretical models were employed to validate the experimental findings, providing deeper insights into the behavior of cumene-propanone-2 binary liquid mixtures.

2.6. Calculation of acoustic and thermodynamic parameters

Using the experimentally measured values of ultrasonic velocity (U), density (ρ), and viscosity (η), various acoustic and thermodynamic parameters were calculated using the following equations:

1. Isentropic Compressibility (κ_s):

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

2. Intermolecular Free Length (L_f):

$$L_f = K \cdot \sqrt{\kappa_s}$$

3. Molar Volume (V_m):

$$V_m = \frac{M}{\rho}$$

4. Available Volume (V_a):

$$V_a = V_t - V_m$$

Where V_t is the theoretical molar volume based on ideal mixing.

$$\tau = \frac{4\eta}{3\rho U^2}$$

6. Acoustic Impedance (Z):

$$Z = \rho \cdot U$$

7. Excess Parameters:

$$A^E = A_{\text{observed}} - A_{\text{ideal}}$$

2.5. Data Visualization

To ensure a robust and comprehensive analysis of the experimental results, a systematic approach to data analysis and visualization was employed. The collected data were first organized into tabulated formats, providing clear and concise records for further evaluation. Graphical representations were then created to identify trends, deviations, and patterns that would not be immediately evident from raw data alone. This visual approach allowed for easier interpretation of the results, highlighting key relationships between temperature, concentration, and other relevant variables.

Statistical tools were used extensively to analyze the experimental data. This included performing statistical tests to assess the significance of any deviations observed from the ideal mixing behavior. By comparing experimental results against theoretical predictions, the study was able to highlight areas of non-ideal behavior, which is crucial in understanding the underlying thermodynamic processes. The application of these statistical methods helped to validate the consistency of the results and ensure their reliability.

Furthermore, the findings were critically compared to existing literature data for similar systems, which provided an additional layer of verification. This comparison not only confirmed the accuracy of the current study's results but also helped to position the findings within the broader context of the field. By ensuring that the results aligned with established data, the study's conclusions were further solidified, providing a solid foundation for future research on non-ideal mixing behavior in thermodynamic modeling.

This comprehensive approach to data analysis and visualization allowed for meaningful conclusions to be drawn from the experimental data, contributing valuable insights to the understanding of non-ideal mixing behaviors. The study's methodology, with its emphasis on rigor and reproducibility, provides a reliable framework for further investigations in this area.

3. Results

3.1. Ultrasonic Velocity, Density, and Viscosity

- **Ultrasonic Velocity (U):** The ultrasonic velocity increased with the increasing mole fraction of cumene, suggesting stronger intermolecular interactions. Specifically, dipole-dipole interactions between cumene's methyl groups and propanone-2's carbonyl group are responsible for this increase. A decrease in ultrasonic velocity was observed with rising temperature, indicating that higher temperatures weaken the intermolecular forces due to increased molecular motion.
- **Density (ρ):** Density values showed a gradual increase with increasing mole fraction of cumene, consistent with the higher molecular weight and compact structure of cumene. However, density decreased with rising temperature, reflecting thermal expansion and reduced molecular packing efficiency.
- **Viscosity (η):** Viscosity increased with higher mole fractions of cumene, indicating stronger interaction forces in the mixture. A decrease in viscosity with rising temperature suggests reduced intermolecular friction under higher thermal conditions.

3.2. Acoustic and Thermodynamic Parameters

- **Isentropic Compressibility (κ_s):** The isentropic compressibility decreased with increasing mole fraction of cumene, indicating stronger molecular interactions. This trend was more pronounced at lower temperatures, where the intermolecular forces were stronger.
- **Intermolecular Free Length (L_f):** The intermolecular free length followed a similar trend to compressibility, decreasing with higher mole fractions. Elevated temperatures increased the free length, indicating reduced molecular cohesion.
- **Molar Volume (V_m) and Available Volume (V_a):** Molar volume values increased slightly with increasing mole fraction, while available volume decreased. These opposing trends suggest densification of the molecular network at higher cumene concentrations. Negative deviations in excess molar volume (V_m^E) and available volume (V_a^E) indicate non-ideal mixing behavior.
- **Relaxation Time (τ):** Relaxation time increased with mole fraction, reflecting enhanced energy transfer efficiency due to stronger molecular interactions. A decline in relaxation time at elevated temperatures corresponds to reduced viscous drag.
- **Acoustic Impedance (Z):** Acoustic impedance showed a positive correlation with mole fraction, signifying an increase in the density-velocity product. This reinforces the presence of stronger intermolecular interactions, especially at lower temperatures.

3.3. Excess Properties

- **Excess Compressibility (κ_s^E):** Negative excess compressibility values were observed at all temperatures, with higher magnitudes at lower temperatures, confirming significant molecular interactions that lead to a denser liquid structure.
- **Excess Free Length (L_f^E):** Negative excess free length values corroborated strong dipole-dipole interactions. The magnitude of these values decreased with rising temperature, suggesting diminishing interaction strength.
- **Excess Molar Volume (V_m^E):** Negative excess molar volume values indicated effective molecular packing, driven by favorable interactions between cumene and propanone-2.

3.4. Temperature Dependence of Interactions

- At **303 K**, stronger intermolecular interactions were observed due to reduced kinetic energy and increased molecular cohesion.
- As temperature increased to **308 K** and **313 K**, weaker interactions were evident, manifested as reduced ultrasonic velocity, higher compressibility, and increased free length. These trends correspond to thermal disruption of molecular interactions.

3.5. Molecular Interaction Mechanism

- Dipole-dipole interactions are the primary molecular forces at play, with cumene's methyl groups forming hydrogen bonds with the carbonyl oxygen in propanone-2. These interactions result in a structured molecular network, which becomes weaker at higher temperatures due to thermal agitation.

3.6. Comparison with Literature

- The trends observed in this study align with similar studies on polar binary systems, such as those reported by Patil and Naik (2015) and Kolhe and Bhosale (2017). These

studies also highlighted the impact of temperature and composition on ultrasonic and thermodynamic properties.

4. Discussion

The results presented in this study provide valuable insights into the molecular interactions in binary mixtures of cumene and propanone-2, with a particular focus on how temperature and composition influence the physical properties of the mixtures.

4.1. Molecular Interactions

The **increase in ultrasonic velocity** with the mole fraction of cumene points to the strengthening of intermolecular forces, particularly dipole-dipole interactions between cumene's methyl groups and propanone-2's carbonyl group. This trend was further confirmed by the **increase in viscosity** with higher mole fractions, suggesting enhanced intermolecular friction and stronger interactions. Conversely, the **decrease in ultrasonic velocity** and **viscosity** at elevated temperatures indicates that thermal energy weakens these interactions, which is in line with the behaviour of many polar molecular systems where intermolecular forces are disrupted by heat.

The observation of a **decrease in density** with temperature is also expected, as thermal expansion leads to a reduction in molecular packing efficiency. This was further supported by the trend in **molar volume and available volume**, where the increase in molar volume with mole fraction and the decrease in available volume suggested densification of the molecular network, which is consistent with the favourable interactions between cumene and propanone-2.

4.2. Temperature Effects

The **temperature dependence** of the parameters demonstrated the expected trend where lower temperatures (303 K) facilitated stronger molecular interactions, as evidenced by the decreased free length and compressibility. At higher temperatures (308 K and 313 K), the weakening of intermolecular forces was evident, leading to increased free length and compressibility. These findings align with the general principle that increasing temperature leads to the disruption of intermolecular interactions due to increased molecular motion.

4.3. Acoustic and Thermodynamic Parameters

The derived **acoustic and thermodynamic parameters** such as isentropic compressibility, relaxation time, and acoustic impedance offer deeper insights into the nature of the molecular interactions. The negative excess values of compressibility and free length at all temperatures highlight the non-ideal mixing behaviour of the system, with molecular interactions playing a dominant role. The observed trends in **relaxation time** also align with the viscosity data, further confirming the role of temperature in modulating molecular dynamics.

4.4. Molecular Interaction Mechanism

The molecular interactions in these mixtures appear to be dominated by **dipole-dipole forces**, with cumene's methyl groups forming hydrogen bonds with the carbonyl group of propanone-2. This mechanism aligns with the negative deviations in excess properties, which are characteristic of systems with specific intermolecular interactions.

4.5. Comparison with Previous Studies

When compared with the literature, such as studies by Patil and Naik (2015) and Kolhe and Bhosale (2017), the trends observed here are consistent with previous research on polar binary mixtures. The current study extends these findings by providing a more detailed analysis of cumene-propanone-2 mixtures, adding a new perspective on the temperature dependence and molecular interactions in these systems.

4.6. Practical Implications

Understanding the molecular interactions in polar liquid mixtures has significant implications for a range of industries, including chemical process design and pharmaceutical formulations. The temperature-dependent behaviour of these systems provides valuable information for optimizing processes that involve such mixtures, particularly in areas where viscosity and molecular packing play crucial roles, such as in the design of solvents or reaction media.

5. Conclusion

This work thoroughly examined the molecular interactions in binary mixtures of cumene and propanone-2 by ultrasonic velocity, density, and viscosity measurements, as well as derived acoustic and thermodynamic characteristics. The findings indicate substantial dipole-dipole and hydrogen-bonding interactions, resulting in non-ideal mixing behavior. The noted negative deviations in excess characteristics suggest robust associative associations, especially at reduced temperatures. Temperature-dependent fluctuations in acoustic and thermodynamic parameters validate the attenuation of molecular interactions with elevated thermal energy. The results correspond with prior studies on analogous systems and offer significant insights for applications in industrial formulations, materials science, and chemical process design. Future research may concentrate on expanding the study to ternary systems or integrating spectroscopic methods for further validation of interaction processes. The research offers essential insights into molecular interactions within polar liquid mixtures, impacting areas such as chemical process design, material production, and industrial formulations. Comprehending the temperature-dependent behaviour of these systems provides essential insights for enhancing processes in the chemical and pharmaceutical sectors.

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