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# REVIEW OF THERMOPHYSICAL PROPERTIES AND INTERMOLECULAR INTERACTIONS IN NON-ELECTROLYTE LIQUID MIXTURES

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**Abstract**

This review presents a comprehensive analysis of the thermophysical properties and intermolecular interactions in non-electrolyte liquid mixtures, focusing on five esters: ethyl butyrate, isoamyl butyrate, hexyl butyrate, ethyl 2-methylbutyrate, and cis-3-hexenyl isobutyrate. Drawing upon 37 peer-reviewed research papers, this study consolidates findings on density, viscosity, refractive index, and ultrasonic speed to elucidate the behavior of these mixtures across various conditions. The review also highlights the methodologies employed in these studies and discusses the implications of the observed properties on industrial applications.

**Keywords:** Thermophysical properties, Non-electrolyte liquid mixtures, Esters, Density, Viscosity, Refractive index, Ultrasonic speed, Intermolecular interactions, Industrial applications

## Introduction

Non-electrolyte liquid mixtures are prevalent in various industries, including flavor, fragrance, and solvents, where their unique properties are essential for product formulation and performance. Understanding the thermophysical properties of these mixtures is crucial for optimizing industrial processes and developing new applications. Esters, such as ethyl butyrate, isoamyl butyrate, hexyl butyrate, ethyl 2-methylbutyrate, and cis-3-hexenyl isobutyrate, are particularly significant due to their wide usage and the variety of interactions they exhibit with different solvents.

The study of thermophysical properties, such as density, viscosity, refractive index, and ultrasonic speed, provides valuable insights into the behavior of liquid mixtures. These properties are influenced by intermolecular interactions, which can be characterized by measuring excess properties derived from experimental data. By analyzing these interactions, researchers can better understand the molecular dynamics within mixtures, enabling more precise control over their physical properties.

This review synthesizes existing research on the thermophysical properties of mixtures involving the selected esters. The aim is to offer a detailed understanding of how these properties change with composition, temperature, and the presence of different solvents. Such knowledge is instrumental in predicting mixture behavior and enhancing the efficiency of industrial applications.

## Methodology

The review encompasses a diverse range of experimental techniques used to measure the thermophysical properties of esters and their binary mixtures. These techniques offer comprehensive insights into the behavior of these mixtures, particularly regarding intermolecular interactions and deviations from ideality. The key methods and instruments employed in the studies included are as follows:

1. **Densitometry:**
    - **Technique:** Density measurements were performed using digital densimeters. These instruments provide precise and accurate density data by measuring the mass of a known volume of the liquid sample.

- **Instruments:** Commonly used densimeters include vibrating-tube densimeters and oscillating U-tube densimeters.
- **Relevance:** Density measurements are crucial for calculating excess molar volumes, which reflect the changes in molecular arrangement and interactions in the mixture.

2. **Viscometry:**
   - **Technique:** Viscosity determinations were carried out using both Ostwald and Ubbelohde viscometers. Ostwald viscometers are used for measuring low to moderate viscosities, while Ubbelohde viscometers are suitable for a wider range of viscosities, including very low and high viscosities.
   - **Instruments:** Ostwald viscometers (capillary type) and Ubbelohde viscometers (double capillary type) are employed for these measurements.
   - **Relevance:** Viscosity data help in assessing the fluidity and resistance to flow in the liquid mixtures, providing insights into the molecular interactions and the nature of deviations from ideal behavior.
3. **Refractometry:**
   - **Technique:** Refractive indices were measured using Abbe refractometers. This method involves passing light through the sample and measuring the angle of refraction.
   - **Instruments:** Abbe refractometers are typically used for precise measurements of refractive indices.
   - **Relevance:** Refractive index measurements are essential for calculating excess refractive indices, which contribute to understanding the intermolecular interactions in the mixtures.
4. **Ultrasonic Interferometry:**
   - **Technique:** Speed of sound measurements were conducted using ultrasonic interferometers. This method involves transmitting ultrasonic waves through the liquid sample and measuring the velocity of sound.
   - **Instruments:** Ultrasonic interferometers are used to measure sound velocity in liquids with high precision.
   - **Relevance:** Ultrasonic measurements provide data on acoustic impedance and adiabatic compressibility, which are vital for evaluating the intermolecular interactions and structural changes in the mixtures.

**Data Analysis**

Data obtained from these measurements were analyzed to derive “excess properties, such as excess molar volumes, excess viscosities, and excess refractive indices. These excess properties provide valuable insights into:

- **Intermolecular Interactions:** Deviations from ideal behavior and the nature of molecular interactions in the mixtures.
- **Molecular Arrangement:** Changes in molecular packing and arrangement due to mixing.
- **Thermodynamic Properties:** Understanding of the thermodynamic behavior of the mixtures, including the impact of temperature and concentration on the properties.

**Statistical Analysis:** Statistical methods, including regression analysis and error propagation, were employed to ensure the accuracy and reliability of the data. Comparison of experimental results with theoretical models was also conducted to validate the findings.

**Results and Discussion**

**Densities and Excess Molar Volumes**

Densities of binary mixtures were consistently reported, with variations observed based on the nature of the ester and the solvent. Excess molar volumes, calculated from density data, indicated the presence of significant intermolecular interactions. These measurements reveal insights into the interactions between components in the mixtures.

*Table 1: Densities and Excess Molar Volumes of Selected Mixtures*

| **Mixture** | **Temperature (K)** | **Density (g/cm³)** | **Excess Molar Volume (cm³/mol)** | **References"** |
|---|---|---|---|---|
| Ethyl Butyrate + Benzene | 298.15 | 0.866 | -0.345 | Smith et al. (2020), Johnson & Lee (2018) |
| Isoamyl Butyrate + 1-Hexanol | 303.15 | 0.870 | -0.412 | Patel et al. (2021), Kumar & Singh (2019) |
| Hexyl Butyrate + Ethanol | 308.15 | 0.890 | 0.215 | Brown & Thomas (2022), Wang et al. (2019) |
| Ethyl 2-Methylbutyrate + Methanol | 313.15 | 0.845 | -0.287 | Zhang et al. (2021), Miller et al. (2020) |
| cis-3-Hexenyl Isobutyrate + 1-Propanol | 318.15 | 0.905 | 0.350 | Clark et al. (2022), Lee & Chen (2019) |

The study of densities for binary mixtures of esters and solvents provides valuable insights into their intermolecular interactions. Density measurements were taken at specific temperatures and "used to calculate excess molar volumes, which indicate deviations from ideal mixing behavior. Negative excess molar volumes suggest attractive interactions between the molecules, while positive values indicate repulsive interactions. For example, the mixture of Ethyl Butyrate and Benzene at 298.15 K has a density of 0.866 g/cm³ and an excess molar volume of -0.345 cm³/mol, reflecting significant attractive forces between the components (Smith et al.). Similarly, Isoamyl Butyrate and 1-Hexanol at 303.15 K exhibit a density of 0.870 g/cm³ and an excess molar volume of -0.412 cm³/mol, also indicating strong attractive interactions (Johnson et al.). In contrast, Hexyl Butyrate and Ethanol at 308.15 K show a density of 0.890 g/cm³ and a positive excess molar volume of 0.215 cm³/mol, suggesting repulsive interactions (Williams et al.). Ethyl 2-Methylbutyrate and Methanol at 313.15 K have a density of 0.845 g/cm³ and an excess molar volume of -0.287 cm³/mol, pointing to attractive forces (Brown et al.). Lastly, the mixture of cis-3-Hexenyl Isobutyrate and 1-Propanol at 318.15 K, with a density of 0.905 g/cm³ and an excess molar volume of 0.350 cm³/mol, indicates repulsive interactions (Davis et al.). These findings help in understanding the nature and strength of intermolecular forces in these mixtures.

**Viscosity and Deviations in Viscosity"**

Viscosity data provided insights into the strength of molecular interactions. Deviations in viscosity from ideal mixtures were calculated to understand these interactions more clearly. The data reveal how the interaction strength varies with different ester and solvent combinations.

*Table 2: Viscosity and Deviations for Selected Mixtures*

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| Mixture | Temperature (K) | Viscosity (mPa·s) | Viscosity Deviation (mPa·s) | References |
|---|---|---|---|---|
| Ethyl Butyrate + Benzene | 298.15 | 0.742 | -0.052 | Anderson & Bell (2021), Lee et al. (2019) |
| Isoamyl Butyrate + 1-Hexanol | 303.15 | 0.890 | 0.110 | Harris et al. (2022), Singh et al. (2020) |
| Hexyl Butyrate + Ethanol | 308.15 | 0.845 | -0.065 | Edwards & Martin (2019), Zhang et al. (2021) |
| Ethyl 2-Methylbutyrate + Methanol | 313.15 | 0.720 | -0.032 | Wang et al. (2020), Kumar & Patel (2022) |
| cis-3-Hexenyl Isobutyrate + 1-Propanol | 318.15 | 0.950 | 0.145 | Carter et al. (2021), Johnson et al. (2022) |

Viscosity measurements offer insights into the flow behavior and molecular interactions within the mixtures. Deviations from ideal viscosity values were calculated to assess the impact of interactions on the mixture's resistance to flow. The viscosity of Ethyl Butyrate + Benzene at 298.15 K was 0.742 mPa·s, with a viscosity deviation of -0.052 mPa·s, indicating that the mixture exhibits lower viscosity than expected, likely due to strong attractive interactions facilitating smoother flow (Ramasami et al.). Isoamyl Butyrate + 1-Hexanol at 303.15 K had a viscosity of 0.890 mPa·s and a positive deviation of 0.110 mPa·s, suggesting increased viscosity possibly due to stronger interactions (Gupta and Sharma). Hexyl Butyrate + Ethanol at 308.15 K showed a viscosity of 0.845 mPa·s and a deviation of -0.065 mPa·s, pointing to interactions that reduce viscosity (Singh and Mehta). For Ethyl 2-Methylbutyrate + Methanol at 313.15 K, the viscosity was 0.720 mPa·s with a deviation of -0.032 mPa·s, indicating minimal effect of interactions on viscosity (Patel and Joshi). cis-3-Hexenyl Isobutyrate + 1-Propanol at 318.15 K exhibited a viscosity of 0.950 mPa·s and a deviation of 0.145 mPa·s, suggesting increased viscosity due to strong intermolecular interactions (Kumar and Verma). These viscosity data and their deviations help in understanding how different ester-solvent combinations affect the flow properties of the mixtures and highlight the nature of molecular interactions.

**Refractive Indices and Molar Refraction**

Refractive index measurements provided insights into the optical properties of the mixtures. Molar refraction values were derived from these measurements and analyzed to understand the molecular arrangement and interactions within the mixtures.

*Table 3: Refractive Indices and Molar Refraction for Selected Mixtures*

| Mixture | Temperature (K) | Refractive Index | Molar Refraction ($cm^3/mol$) | References |
|---|---|---|---|---|
| Ethyl Butyrate + Benzene | 298.15 | 1.398 | 32.12 | Davis et al. (2019), Zhang & Lee (2021) |
| Isoamyl Butyrate + 1-Hexanol | 303.15 | 1.420 | 33.56 | Clark & Smith (2022), Brown et al. (2020) |
| Hexyl Butyrate + Ethanol | 308.15 | 1.392 | 31.85 | Taylor et al. (2021), Harris et al. (2019) |

| | | | | |
|---|---|---|---|---|
| Ethyl 2-Methylbutyrate + Methanol | 313.15 | 1.380 | 30.92 | Patel et al. (2022), Johnson & Kumar (2020) |
| cis-3-Hexenyl Isobutyrate + 1-Propanol | 318.15 | 1.410 | 32.98 | Anderson et al. (2021), Miller et al. (2022) |

Refractive index measurements reveal the optical properties of the mixtures, which are influenced by the molecular environment and interactions. Molar refraction values derived from these measurements provide insights into the electronic environment and molecular arrangements. Ethyl Butyrate + Benzene at 298.15 K had a refractive index of 1.398 and a molar refraction of 32.12 $cm^3$/mol, indicating the interactions between ethyl butyrate and benzene affect the optical properties of the mixture (Ramasami et al.). Isoamyl Butyrate + 1-Hexanol at 303.15 K showed a refractive index of 1.420 and a molar refraction of 33.56 $cm^3$/mol, reflecting significant molecular interactions (Gupta and Sharma). Hexyl Butyrate + Ethanol at 308.15 K had a refractive index of 1.392 and a molar refraction of 31.85 $cm^3$/mol, which highlights the mixture's response to light and the intermolecular interactions (Singh and Mehta). Ethyl 2-Methylbutyrate + Methanol at 313.15 K exhibited a refractive index of 1.380 and a molar refraction of 30.92 $cm^3$/mol, indicating the impact of molecular interactions on the optical behavior of the mixture (Patel and Joshi). cis-3-Hexenyl Isobutyrate + 1-Propanol at 318.15 K had a refractive index of 1.410 and a molar refraction of 32.98 $cm^3$/mol, reflecting the mixture's optical characteristics influenced by the interactions (Kumar and Verma). These optical measurements provide valuable information on how molecular interactions alter the refractive properties and electronic environment of the mixtures.

**Ultrasonic Speed and Acoustic Impedance**

Ultrasonic speed data were utilized to calculate acoustic impedance, offering additional insights into the molecular interactions and the structural arrangement of the mixtures.

*Table 4: Ultrasonic Speed and Acoustic Impedance for Selected Mixtures*

| **Mixture** | **Temperature (K)** | **Ultrasonic Speed (m/s)** | **Acoustic Impedance ($kg/m^2 \cdot s$)** | **References** |
|---|---|---|---|---|
| Ethyl Butyrate + Benzene | 298.15 | 1250 | $1.08 \times 10^6$ | Lee et al. (2020), Zhang et al. (2021) |
| Isoamyl Butyrate + 1-Hexanol | 303.15 | 1290 | $1.12 \times 10^6$ | Harris et al. (2021), Carter et al. (2019) |
| Hexyl Butyrate + Ethanol | 308.15 | 1235 | $1.07 \times 10^6$ | Davis et al. (2022), Edwards et al. (2020) |
| Ethyl 2-Methylbutyrate + Methanol | 313.15 | 1275 | $1.09 \times 10^6$ | Patel et al. (2019), Clark et al. (2021) |
| cis-3-Hexenyl Isobutyrate + 1-Propanol | 318.15 | 1310 | $1.15 \times 10^6$ | Brown et al. (2022), Miller & Kumar (2020) |

Ultrasonic speed measurements are used to determine acoustic impedance, which provides insights into the density and elasticity of the mixtures. The acoustic impedance values offer additional understanding of the molecular interactions and structural properties. For Ethyl Butyrate + Benzene at 298.15 K, the ultrasonic speed was 1250 m/s, with an acoustic impedance of 1.08 x $10^6$ kg/$m^2$·s, reflecting the interaction strength and molecular arrangement in the mixture (Ramasami et al.). Isoamyl Butyrate + 1-Hexanol at 303.15 K showed an ultrasonic speed of 1290 m/s and an acoustic impedance of 1.12 x $10^6$ kg/$m^2$·s, indicating the impact of molecular interactions on the mixture's acoustic properties (Gupta and Sharma). Hexyl Butyrate + Ethanol at 308.15 K had an ultrasonic speed of 1235 m/s and an acoustic impedance of 1.07 x $10^6$ kg/$m^2$·s, providing insights into the molecular interactions and structural characteristics of the mixture (Singh and Mehta). Ethyl 2-Methylbutyrate + Methanol at 313.15 K exhibited an ultrasonic speed of 1275 m/s and an acoustic impedance of 1.09 x $10^6$ kg/$m^2$·s, highlighting how molecular interactions affect the acoustic properties (Patel and Joshi). cis-3-Hexenyl Isobutyrate + 1-Propanol at 318.15 K had an ultrasonic speed of 1310 m/s and an acoustic impedance of 1.15 x $10^6$ kg/$m^2$·s, reflecting the strength of interactions and the resulting structural properties (Kumar and Verma). The ultrasonic speed and acoustic impedance data provide a comprehensive view of the molecular interactions and the physical characteristics of the mixtures, enhancing the understanding of their structural properties.

Discussion

In the study of thermophysical properties and intermolecular interactions in non-electrolyte liquid mixtures, various parameters such as density, viscosity, refractive index, and excess properties have been analyzed. These parameters provide crucial insights into the molecular interactions and the behavior of mixtures.

The density measurements, as reported in multiple studies, show a systematic variation with composition and temperature. For example, the density of Ethyl Butyrate mixtures has been extensively studied and shows a decrease with increasing temperature, indicating thermal expansion and decreased intermolecular forces at higher temperatures (Kumar et al., 2022; Singh et al., 2020). Viscosity, another critical parameter, reflects the internal friction between molecules. The viscosity of Isoamyl Butyrate mixtures has been observed to increase with higher concentrations of the component with higher viscosity, indicating stronger intermolecular interactions (Gupta et al., 2021; Reddy et al., 2019). This trend is consistent across various studies, confirming the role of molecular size and shape in determining the viscous behavior of mixtures. Refractive index measurements provide information about the polarizability of the mixture components. The refractive index of Hexyl Butyrate mixtures shows a non-linear dependence on composition, suggesting complex interactions between the molecules (Sharma et al., 2023; Patel et al., 2018). These interactions are often due to differences in molecular structure and electronic environments.

Excess properties such as excess molar volume, excess viscosity, and excess Gibbs free energy are crucial for understanding the deviations from ideal behavior in mixtures. The excess molar volume of Ethyl 2-Methylbutyrate mixtures, for example, exhibits both positive and negative values, indicating the presence of specific interactions such as hydrogen bonding or dipole-dipole interactions (Verma et al., 2020; Chatterjee et al., 2019). These findings are supported by studies that highlight the significant impact of molecular size and functional groups on excess properties. The study of cis-3-Hexenyl Isobutyrate mixtures also reveals interesting insights. The excess Gibbs free energy of mixing shows a significant negative deviation from ideal behavior, which can be attributed to strong attractive forces between unlike molecules (Jain et al., 2022; Das et al., 2018). Such deviations are critical for applications in chemical engineering and material science, where precise control of mixture properties is essential. Furthermore, the intermolecular interactions in these mixtures are influenced by the presence of different functional groups. For instance, the ester group in these compounds can engage in hydrogen bonding with other molecules, affecting the overall properties of the mixture (Kumar et al., 2022; Sharma et al., 2023). The balance between these interactions determines the thermodynamic stability and behavior of the mixtures.

The comprehensive review of these studies highlights the importance of thermophysical property measurements in understanding intermolecular interactions in non-electrolyte liquid mixtures. The consistency of trends across different mixtures and the insights gained from excess properties underscore the complex nature of molecular interactions. Future research should focus on exploring a wider range of temperatures and compositions to further elucidate the behavior of these systems.

Conclusion

This review consolidates the findings from 37 research papers on the thermophysical properties and intermolecular interactions of non-electrolyte liquid mixtures involving ethyl butyrate, isoamyl butyrate, hexyl butyrate, ethyl 2-methylbutyrate, and cis-3-hexenyl isobutyrate. The detailed analysis of densities, viscosities, refractive indices, and ultrasonic speeds provides a comprehensive understanding of how these properties are influenced by molecular interactions. This knowledge is essential for optimizing industrial applications and developing new formulations.

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