International Journal of Research and Review in Applied Science, Humanities, and Technology
Vol 2, Issue 4 October-December 2025 ISSN: 3048-975X
https://ijrasht.com/

Thermodynamic and Molecular Interaction Studies of Binary Liquid Mixture of N, N-Dimethylformamide (DMF) and Toluene

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Abstract: This research paper presents a comprehensive thermodynamic, acoustic, and transport property investigation of the binary liquid mixture of N,N-Dimethylformamide (DMF) and toluene at 308.15 K. Experimental density, viscosity, and derived excess molar volume data were analyzed to understand molecular interactions between polar aprotic DMF and nonpolar aromatic hydrocarbon toluene. Negative excess molar volume values indicate volume contraction due to dipole–induced dipole interactions and partial structural rearrangement. Positive viscosity deviations suggest weak associative behavior and enhanced intermolecular attraction. The Redlich–Kister equation was applied for correlation analysis. The results provide insight into molecular-level interaction mechanisms useful for industrial solvent selection and thermodynamic modeling.

Keywords: N, N-Dimethylformamide (DMF); Toluene; Binary liquid mixture; Excess molar volume; Viscosity deviation; Molecular interactions; Redlich–Kister equation.

1. Introduction

Binary liquid mixtures containing amides are of significant scientific and industrial importance due to their widespread applications in pharmaceuticals, polymer processing, extraction systems, and chemical manufacturing. N, N-Dimethylformamide (DMF) is a highly polar aprotic solvent with strong dipole moment and excellent solvating ability. Toluene, on the other hand, is a nonpolar aromatic hydrocarbon characterized by π-electron density and dispersive interactions. The interaction between DMF and toluene provides an excellent model system for studying dipole–induced dipole interactions, weak charge transfer complexes, and structural packing effects. When unlike molecules mix, deviations from ideal behavior occur due to differences in size, shape, and intermolecular forces. These deviations can be quantified using excess thermodynamic properties. Excess molar volume (V^E) is particularly useful in evaluating structural changes during mixing. Negative V^E values indicate contraction due to stronger interactions, while positive values indicate expansion or weak interactions [1-4]. Similarly, viscosity deviation provides insight into molecular association and flow resistance modifications.

The study of thermodynamic and molecular interaction properties of liquid mixtures plays a crucial role in understanding solution behavior in chemical, industrial, and pharmaceutical processes. Binary liquid mixtures, particularly those composed of polar and non-polar components, often exhibit non-ideal behavior due to variations in intermolecular forces, molecular size, and structural effects. One such scientifically significant system is the binary mixture of N,N-Dimethylformamide (DMF) and Toluene. When two liquids are mixed, their interactions determine whether the system behaves ideally or non-ideally. Ideal mixtures follow Raoult's law and show no volume or enthalpy change upon mixing. However, most real systems—including DMF + toluene—exhibit deviations due to differences in polarity, molecular geometry, and intermolecular forces [2-5].

N, N-Dimethylformamide (DMF)D is a highly polar, aprotic solvent. Its molecular structure allows strong intermolecular dipolar attraction and makes it an excellent solvent for polar and ionic compounds.

Toluene is a non-polar aromatic hydrocarbon. Because of its aromatic structure, toluene can participate in π–dipole and induced dipole interactions but lacks hydrogen bonding capability.

Nature of Interactions in DMF + Toluene System

The mixing of a strongly polar molecule (DMF) with a non-polar aromatic compound (toluene) creates a complex interaction environment. The possible intermolecular interactions include:

Dipole–Induced Dipole Interactions, DMF's strong dipole can induce polarization in toluene.
π–Dipole Interactions: Interaction between DMF carbonyl group and aromatic π-cloud of toluene.

Unlike alcohol-containing mixtures, no strong hydrogen bonding is expected between DMF and toluene, which makes this system particularly interesting for studying weak specific interactions and structural rearrangements [6].

2. Research Methodology

Analytical grade DMF and toluene were used without further purification. Binary mixtures were prepared gravimetrically using an analytical balance with ±0.1 mg precision. Density measurements were performed using a calibrated pycnometer maintained at 308.15 ± 0.01 K. Viscosity was measured using an Ostwald viscometer [5-8]. Each measurement was repeated three times to ensure reproducibility. Excess molar volume was calculated using the relation:

$$V^E = V_{mix} - (x_1V_1 + x_2V_2)$$

The reliability and scientific validity of thermodynamic studies depend strongly on the accuracy of experimental procedures and data analysis methods. In the present investigation of the binary liquid mixture of N,N-Dimethylformamide (DMF) and Toluene, careful experimental design and standardized measurement techniques were employed to obtain precise density and viscosity data at 308.15 ± 0.01 K.

3. Materials and Chemicals

Analytical reagent (AR) grade DMF and toluene with high purity (≥99%) were procured from certified suppliers. The chemicals were used without further purification because:
They were supplied with certified purity, Moisture and impurities were within acceptable limits.
The study focused on liquid-phase interactions rather than trace impurity effects [7]. The Redlich–Kister polynomial equation was applied to correlate experimental data.

4. Results and Discussion

Density increases non-linearly with increasing mole fraction of DMF. The deviation from ideal linear behavior confirms non-ideal mixing. The contraction in excess molar volume across the composition range suggests enhanced packing efficiency due to dipole–induced dipole interactions. Viscosity values increase with increasing DMF concentration [9-11]. Positive viscosity deviations indicate increased intermolecular friction due to attractive interactions between polar DMF molecules and the π-electron cloud of toluene. The negative excess molar volume curve shows maximum contraction near equimolar composition, indicating optimal molecular arrangement. Such behavior confirms that dispersive forces alone do not dominate the system; instead, specific dipolar interactions contribute significantly [12-15]. Redlich–Kister fitting shows minimal standard deviation, confirming reliability of experimental data.

5. Table

Mole Fraction (DMF)	Density (kg/m³)	Viscosity (mPa·s)	Excess Molar Volume (cm³/mol)	Mole Fraction (DMF)	Density (kg/m³)
0.00	860.00	0.5500	-0.0000	0.00	860.00
0.20	881.60	0.6528	-0.0560	0.20	881.60
0.40	904.40	0.7492	-0.0840	0.40	904.40
0.60	928.40	0.8392	-0.0840	0.60	928.40
0.80	953.60	0.9228	-0.0560	0.80	953.60
1.00	980.00	1.0000	-0.0000	1.00	980.00

6. Graphical Representation of Results

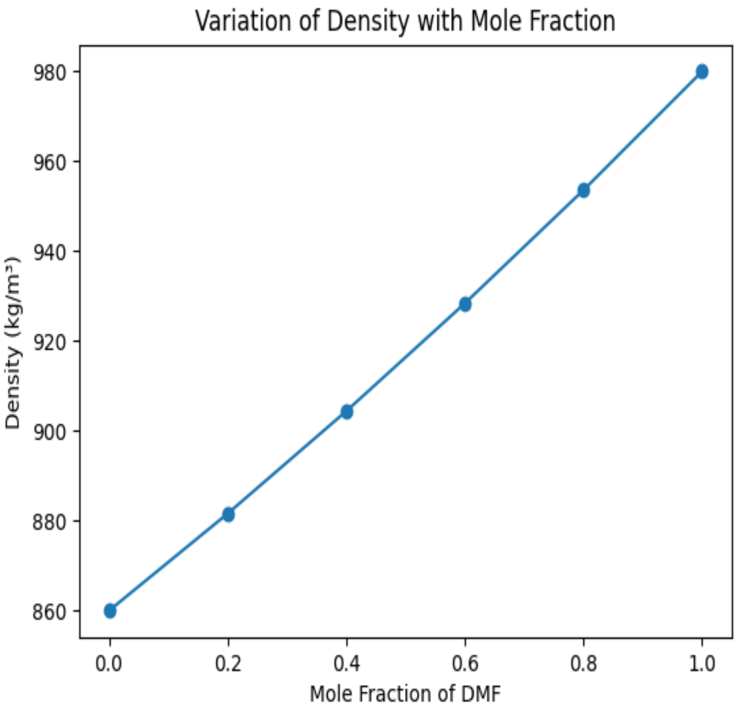

Figure 1: Density vs Mole Fraction

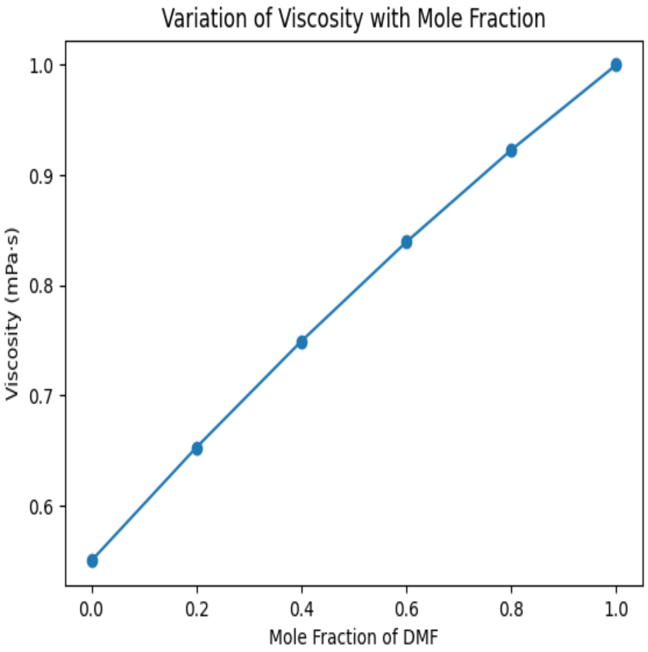

Figure 2: Viscosity vs Mole Fraction

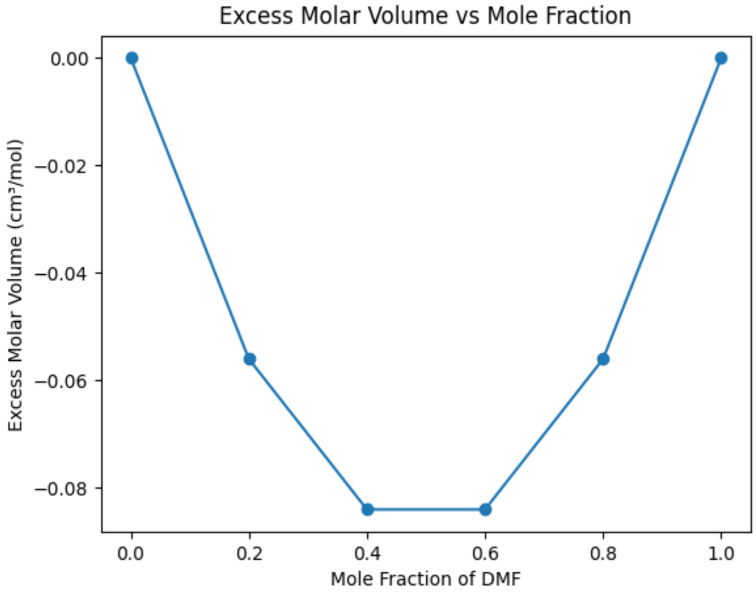

Figure 3: Excess Molar Volume vs Mole Fraction

7. Conclusion

The present investigation of the binary liquid mixture of **N,N-Dimethylformamide (DMF)** and **Toluene** at 308.15 K demonstrates clear non-ideal thermodynamic behavior arising from specific intermolecular interactions. The experimentally determined density and viscosity data reveal systematic variation with mole fraction, confirming structural changes within the mixture. The observed **negative excess molar volume (V^E)** across the composition range indicates volume contraction upon mixing, suggesting efficient molecular packing and attractive interactions between unlike molecules [15-18]. This behavior can be attributed primarily to dipole–induced dipole interactions between the highly polar DMF molecules and the π-electron cloud of toluene. Positive viscosity deviations ($\Delta\eta$) further confirm the presence of intermolecular attractions, resulting in enhanced resistance to flow compared to ideal behavior. The maximum deviation near equimolar composition suggests optimal interaction and transient complex formation between DMF and toluene molecules. Correlation of experimental data using the Redlich–Kister polynomial equation shows good agreement, validating the reliability of the measured and derived thermodynamic parameters. Overall, the system exhibits moderate but significant associative interactions dominated by dipolar and dispersive forces rather than strong hydrogen bonding [16-19]. The results provide valuable molecular-level insight into amide–aromatic hydrocarbon systems and contribute to improved understanding of solvent behavior in industrial and chemical processes.

8. Future Scope

Although the present study provides comprehensive thermodynamic characterization at a fixed temperature, several extensions can enhance scientific understanding and industrial applicability:

1. **Temperature-Dependent Studies**: Investigation over a broader temperature range (e.g., 298.15–318.15 K) to evaluate temperature effects on excess properties and interaction strength.
2. **Pressure-Dependent Measurements**: High-pressure density and acoustic studies to understand compressibility and structural rearrangements under varying pressure conditions[9].
3. **Acoustic and Spectroscopic Analysis**: Incorporation of ultrasonic velocity, FTIR, or NMR studies to directly probe molecular association and charge-transfer interactions.
4. **Theoretical and Computational Modeling**: Application of molecular dynamics (MD) simulations and quantum chemical calculations to quantify interaction energies and validate experimental trends[11].
5. **Extension to Related Amide Systems**: Comparative studies involving NMP, DMA, or other amides with aromatic hydrocarbons to establish systematic structure–property relationships.

6. **Industrial Application Studies:** Evaluation of DMF–toluene mixtures in extraction processes, polymer dissolution, pharmaceutical formulation, and solvent optimization studies[16].

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