

Thermoacoustic Properties of 1-Propanol-*n*-Hexane and 1-Propanol-Cyclohexane Binary Mixtures: A Comparative Study at 298.15 K

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Abstract

*This study reports the measurement of ultrasonic velocity (U), viscosity (η), and density (ρ) for the binary liquid mixtures 1-propanol-*n*-hexane and 1-propanol-cyclohexane at 298.15 K over the full composition range (mole fraction 0.1–0.9). From the experimentally measured data, several important thermodynamic and acoustic parameters, including isentropic compressibility (β_s), acoustic impedance, intermolecular free length, free volume (V_f), and internal pressure (π_i), were systematically derived to assess the magnitude and nature of intermolecular interactions operating within the mixtures. Density, viscosity, and ultrasonic velocity measurements were carried out with high precision using an Anton Paar DSA 5000 M instrument, ensuring reliable and reproducible results across the entire composition range. Comparative analysis revealed that the 1-propanol-cyclohexane system consistently exhibited higher values of ultrasonic velocity, viscosity, acoustic impedance, internal pressure, relaxation behavior, and classical absorption, together with lower isentropic compressibility and intermolecular free length, when compared to the corresponding 1-propanol-*n*-hexane system. These trends clearly indicate enhanced molecular association, reduced free volume, and more efficient molecular packing in mixtures containing cyclohexane. The observed behavior is primarily attributed to the compact, cyclic geometry of cyclohexane, which promotes closer molecular approach and stronger dispersive and associative interactions, in contrast to the relatively flexible linear structure of *n*-hexane. The systematic variation of the evaluated parameters with composition further supports the existence of significant structural rearrangements at the microscopic level. Collectively, the results demonstrate the high sensitivity of ultrasonic and derived acoustic parameters in elucidating microstructural organization and provide a robust and effective framework for probing solute-solvent interactions in mixed liquid systems.*

Keywords: Acoustic impedance, binary liquid mixtures, intermolecular non-covalent interactions, isentropic compressibility, ultrasonic velocity

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Received Date: January 21, 2026

Accepted Date: January 23, 2026

Published Date: February 27, 2026

Citation: Wakulkar A. P., Lanjewar M. R., Shah S. A., Bhukya P. P. Thermoacoustic Properties of 1-Propanol-*n*-Hexane and 1-Propanol-Cyclohexane Binary Mixtures: A Comparative Study at 298.15 K. Journal of Modern Chemistry & Chemical Technology. 2026; 17(1): 19–30p.

INTRODUCTION

A deep understanding of structural characteristics and molecular interactions in liquid mixtures remains vital from theoretical and applied perspectives. Analyzing fundamental thermodynamic and thermo-acoustic properties offers valuable insights into deviations from ideal behavior seen in complex systems. These properties reflect the influence of intermolecular forces like dipole-dipole interactions, van der Waals attractions, and hydrogen bonding between unlike molecules. Beyond scientific significance, they hold practical value, contributing to development of

predictive thermodynamic models essential for improving processes in diverse and global industries, including chemicals, food, pharmaceuticals, petrochemicals, and protective coatings [1,2]. Ultrasonic velocity studies of mixtures comprising polar and non-polar components which are widely utilized in industrial and technological fields, offer a sensitive approach to investigate molecular interactions [3–5]. Acoustic and thermodynamic studies of liquid mixtures provide valuable insights into molecular packing, dynamic behavior, and the strength of intermolecular interactions. Ethanol serves as a key industrial solvent and an essential feedstock for the synthesis of various organic compounds, such as diethyl ether, ethyl halides, acetic acid, esters etc. [6,7]. Owing to its molecular structure, ethanol is frequently regarded as a “universal solvent,” since it can effectively dissolve a wide range of substances, both polar (hydrophilic) and non-polar (hydrophobic) in nature [8]. In the pharmaceutical industry, propanol serves chiefly as a solvent for resins and cellulose esters, with limited application as a disinfectant [9–11]. On the other hand, n-hexane, a non-polar hydrocarbon, is widely used as a recrystallization medium because many organic compounds exhibit high solubility in hot n-hexane but limited solubility at lower temperatures [12,13].

In the present work, molecular interactions in mixtures of polar and non-polar solvents are investigated with particular emphasis on the effect of varying the parent carbon chain. Since the occurrence of hydrogen bonding in mixtures where n-hexane acts as the common component is minimal, the study primarily examines other non-covalent forces that govern the behavior of these systems. Measurements of density (ρ), ultrasonic velocity (U), and viscosity (η) were carried out for the binary mixtures of 1-propanol-n-hexane and 1-propanol-cyclohexane at 298.15 K, across mole fractions ranging from 0.1 to 0.9 to examine the factors responsible for deviations from ideal behavior. Based on experimental data of velocity, viscosity, and density, several derived thermodynamic and acoustic parameters including acoustic impedance, isentropic compressibility, free volume, internal pressure, and free length were evaluated and analyzed to gain insight into the nature of molecular interactions within these mixtures [14,15].

MATERIAL AND METHODS

The objective of this study was to measure ultrasonic velocity (U), viscosity (η), and density (ρ) of binary liquid mixtures at 298.15 K across mole fractions ranging from 0.1 to 0.9 for 1-propanol-n-hexane and 1-propanol-cyclohexane binary systems. From the experimental data, key thermodynamic and acoustic parameters namely isentropic compressibility (β_a), acoustic impedance, free length, free volume (V_f), and internal pressure (π_i) were evaluated. These parameters were further analyzed to provide insights into the strength and nature of intermolecular interactions in the mixtures studied.

The solvents employed were 1-propanol (CAS 71–23-8), n-hexane (CAS 110–54-3), and cyclohexane (CAS 110–82-7) all obtained from Merck KGaA, Darmstadt, Germany, with a minimum purity of 99.8% and used without further purification.

Density, viscosity, and ultrasonic velocity measurements were carried out using an Anton Paar DSA 5000 M instrument. The instrument provides high-precision measurements, with density accurate to ± 0.000007 g cm⁻³ (up to 3 g cm⁻³) and ultrasonic velocity in 1000–2000 m s⁻¹ range with an accuracy of ± 0.01 m s⁻¹, and viscosity over 0.2–30,000 mm² s⁻¹ with an accuracy of $\pm 0.1\%$. The operating temperature spans 0–100°C, with a repeatability of $\pm 0.001^\circ\text{C}$. Measurements are based on the oscillation period of a quartz U-tube containing air, solvent, or the solution under study [16].

Before each run, the U-tube was rinsed with acetone and was subsequently dried by passing moisture-free air through it using an air pump. Drying continued until a constant oscillation period was observed, confirming stability, as performed during the initial calibration of the instrument.

RESULTS AND DISCUSSION

The experimental values of density, ultrasonic velocity, and viscosity for pure 1-propanol, n-hexane and cyclohexane at 298.15 K, together with literature data and standard deviations, are presented in

Table-1. The measured properties of the binary mixtures density (ρ), viscosity (η), and ultrasonic velocity (U) along with the derived thermodynamic and acoustic parameters, namely isentropic compressibility, acoustic impedance, free length, free volume, and internal pressure, are summarized in Tables 2 and 3 for 1-propanol-n-hexane and 1-propanol-cyclohexane systems, respectively. The variations in these parameters are analyzed to gain insight into the molecular interactions present in the mixtures [17–22].

Density is a fundamental physicochemical property reflecting how tightly matter is packed in a given space. It depends on temperature, pressure, and composition, and is directly related to the number of particles per unit volume. When a solute dissolves in solvent, the density of mixture depends on solute-solvent interactions. Strong interactions can compress the molecular structure and increase density, while weak interactions or structural disruption may expand the system and lower density.

Table 1. Thermophysical properties (ρ , u , η) of selected pure liquids at 298.15 K.

298.15 K	Lit	ρ /(g cm ⁻³)	δ	Lit	u /(m s ⁻¹)	δ	Lit	η (mPa.s)	δ
<i>1-Propanol</i>	0.7996	0.799601	1.00×10^{-6}	1205.93	1205.85	0.08	2.1178	2.118	2.0×10^{-4}
<i>n-Hexane</i>	0.65521	0.655214	4.00×10^{-6}	1076.3	1075.72	0.58	0.3036	0.30369	9.0×10^{-5}
<i>Cyclohexane</i>	0.77392	0.77385	7×10^{-5}	1254	1254.03	0.03	0.904	0.89901	4.99×10^{-4}

Table 2. 1-Propanol-n-hexane system.

C (M.F.)	ρ (kg/m ³)	u (m/s ¹)	η (m Pa. s)	$\beta_a \times 10^{-10}$ (cm ² /dyne)	Z (g/cm ² sec)	$L_f \times 10^{-11}$ (cm ² /dyne)	$V_f \times 10^{-8}$ (cm ³ /mol)	$\pi_i \times 10^8$ (dyne/cm ²)	$\tau \times 10^{-13}$ (s)	$a/f^2 \times 10^{-14}$ (sec ² /cm)
0.1	775.85	1180.38	1.6073	9.2508	915797.8	5.9822	3.5291	8.0814	19.825	3.3119
0.2	755.743	1154.59	1.2144	9.9259	872573.3	6.1966	5.5262	6.6553	16.072	2.7449
0.3	736.832	1131.11	0.9323	10.608	833438	6.4059	8.4483	5.5341	13.186	2.2988
0.4	719.617	1114.93	0.7263	11.179	802322.6	6.5762	12.723	4.6346	10.826	1.9147
0.5	704.895	1102.52	0.5719	11.671	777160.8	6.7193	18.907	3.9099	8.8995	1.5917
0.6	691.271	1093.61	0.466	12.096	755980.9	6.8404	26.764	3.3579	7.5157	1.3552
0.7	679.043	1086.19	0.4	12.482	737569.7	6.9489	35.048	2.9652	6.6574	1.2086
0.8	668.909	1081.48	0.3559	12.782	723411.7	7.0318	43.579	2.6711	6.0655	1.106
0.9	660.77	1077.69	0.3241	13.031	712105.2	7.0999	52.312	2.4407	5.6312	1.0304

Table 3. 1-Propanol-cyclohexane system.

C (M.F.)	ρ (kg/m ³)	u (m/s ¹)	η (m Pa.s)	$\beta_a \times 10^{-10}$ (cm ² /dyne)	Z (g/cm ² sec)	$L_f \times 10^{-11}$ (cm ² /dyne)	$V_f \times 10^{-8}$ (cm ³ /mol)	$\pi_i \times 10^8$ (dyne/cm ²)	$\tau \times 10^{-13}$ (s)	$a/f^2 \times 10^{-14}$ (sec ² /cm)
0.1	793.425	1208.87	1.806	8.6245	959147.7	5.7762	3.0562	8.6245	20.768	3.3876
0.2	788.365	1209.53	1.5598	8.6704	953551.1	5.7915	4.0329	7.6348	18.032	2.9398
0.3	784.164	1210.87	1.3784	8.6976	949520.7	5.8006	5.1356	6.8504	15.985	2.6032
0.4	780.823	1213	1.233	8.7041	947138.3	5.8028	6.4152	6.1959	14.31	2.3263
0.5	778.139	1216	1.1186	8.6911	946217	5.7984	7.8413	5.6523	12.962	2.1021
0.6	775.953	1220	1.0299	8.6585	946662.7	5.7875	9.3703	5.2014	11.889	1.9217
0.7	774.177	1225.2	0.9678	8.6049	948521.7	5.7696	10.857	4.841	11.104	1.7871
0.8	772.754	1232	0.9248	8.5258	952032.9	5.743	12.273	4.5471	10.513	1.6828
0.9	771.656	1241.2	0.9004	8.4119	957779.4	5.7045	13.513	4.3127	10.098	1.6043

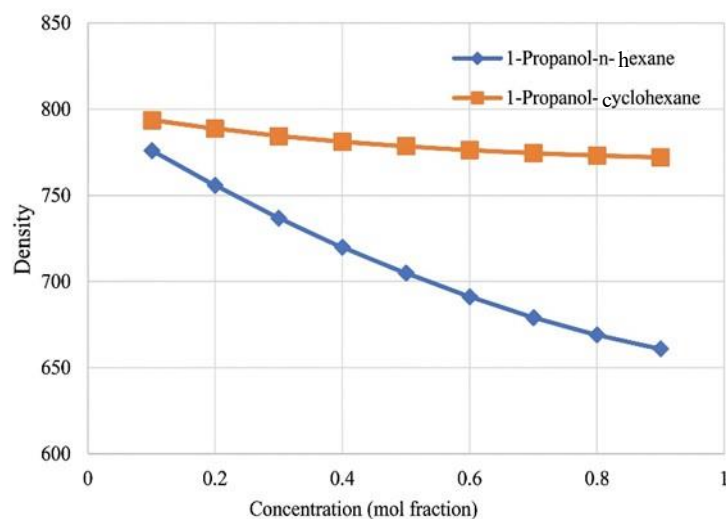


Figure 1. Density vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

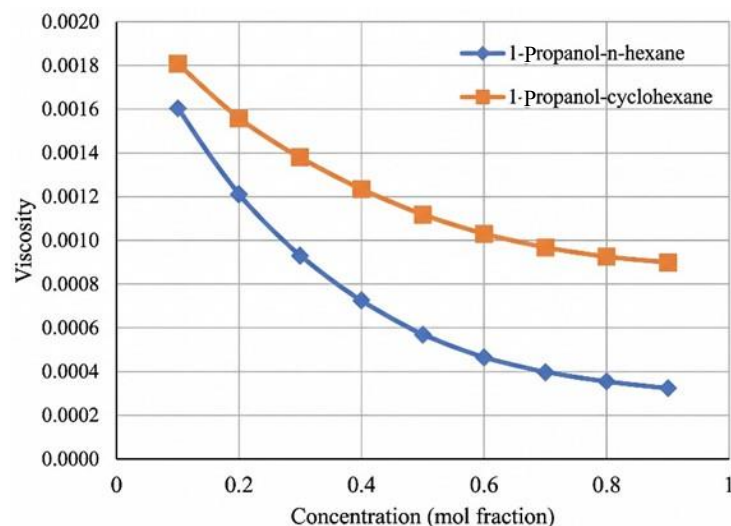


Figure 2. Viscosity vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

From Figure 1, the density of 1-propanol-cyclohexane system is observed to be higher than that of 1-propanol-n-hexane system. This is because cyclohexane is inherently more compact and denser than n-hexane due to its cyclic structure. When mixed with 1-propanol, cyclohexane forms a more efficiently packed mixture, while linear n-hexane produces looser packing. Thus, the higher density of 1-propanol-cyclohexane mixture arises from both the intrinsic density of the cyclic component and the better packing efficiency it provides in the solution [23,24].

The coefficient of viscosity is a key physicochemical property that measures the internal resistance of a liquid to flow. Variations in viscosity arise primarily from the strength and nature of intermolecular interactions, particularly hydrogen bonding and van der Waals forces. An increase in molecular size or solute concentration generally enhances frictional resistance between adjacent liquid layers, leading to higher viscosity. Molecular geometry further modulates viscous behavior. Compact or spherical molecules, typical of branched or cyclic structures tend to orient more uniformly in the direction of flow, thereby minimizing intermolecular obstruction. Conversely, elongated or linear molecules adopt random orientations and impede streamline motion, producing greater resistance and elevated viscosity. Surface area effects follow the same rationale, i.e., molecules with larger exposed surfaces present more extensive intermolecular contact and, therefore, higher frictional drag than those with smaller effective surface areas.

These principles are clearly reflected in the behavior of 1-propanol-cyclohexane and 1-propanol-n-hexane systems which can be observed from Figure 2. Cyclohexane occupies less volume per molecule owing to its cyclic, tightly packed structure thus, more molecules are present in a given volume relative to n-hexane. The reduced intermolecular spacing strengthens van der Waals interactions, increasing the energetic requirement for relative motion. Consequently, cyclohexane, and mixtures containing it exhibit higher viscosity than the corresponding n-hexane solutions [25–29].

Ultrasonic velocity is strongly governed by the intrinsic nature and structural organization of a medium. In general, higher ultrasonic velocities are indicative of enhanced molecular association and tighter packing within the liquid phase. Such associations arise from weak intermolecular forces including van der Waals interactions, hydrogen bonding, dipole-dipole interactions, and dispersion forces which restrict molecular freedom and facilitate faster propagation of ultrasonic waves. Conversely, lower ultrasonic velocities are characteristic of loosely packed molecules and reduced cohesive interactions.

These trends observed from Figure 3 and are evident in the comparative behavior of the 1-propanol-cyclohexane and 1-propanol-n-hexane mixtures. The ultrasonic velocity of the 1-propanol-cyclohexane system is consistently higher than that of the corresponding 1-propanol-n-hexane system. This enhancement may be attributed to the greater density and more compact molecular arrangement within the cyclohexane-containing medium, which favors more efficient transmission of ultrasonic waves [30–32].

Isentropic compressibility serves as an important thermodynamic parameter for probing molecular organization in liquid mixtures. It is defined as the fractional change in volume per unit increase in applied pressure and is directly influenced by the number of free or weakly associated particles present within the system. Because volume is highly sensitive to subtle intermolecular changes, variations in compressibility provide meaningful insight into the extent and nature of molecular interactions including hydrogen bonding, Van der Waals forces, ionic interactions, and hydrophobic association.

In general, pure solvents exhibit higher compressibility than solutions, and compressibility decreases systematically with increasing solute concentration. This reduction reflects enhanced structural organization of the medium. When appreciable solute-solvent interactions occur, molecular packing becomes tighter, reducing the ease with which the system can be compressed. Conversely, weak or negligible interactions, such as those between non-polar solutes and polar solvents lead to less compact arrangements and consequently higher compressibility.

The observed trend in the present study is consistent with these principles. As shown in Figure 4, the isentropic compressibility of the 1-propanol-n-hexane system is higher than that of the 1-propanol-cyclohexane system. The lower compressibility of the cyclohexane containing mixture suggests a more closely packed molecular arrangement and stronger solute-solvent interactions. This behavior arises from the compact cyclic structure of cyclohexane, which permits more efficient packing with 1-propanol molecules relative to the linear n-hexane analogue, thereby increasing molecular association and reducing compressibility [33–36].

Acoustic impedance is defined as the ratio of the instantaneous excess pressure at a point in the medium to the corresponding particle velocity and is determined jointly by the elastic and inertial properties of the system. In liquid mixtures, strong molecular association arising from hydrogen bonding or van der Waals interactions, such as dipole-dipole, dipole-induced dipole, and dispersion forces restrict molecular freedom and increase acoustic impedance.

Intermolecular free length, the average distance between the interacting surfaces of neighboring molecules, behaves analogously to isentropic compressibility. Reduced compressibility corresponds to closer molecular packing and, therefore, a decrease in free length, signaling stronger solute-solvent interactions and denser structural organization.

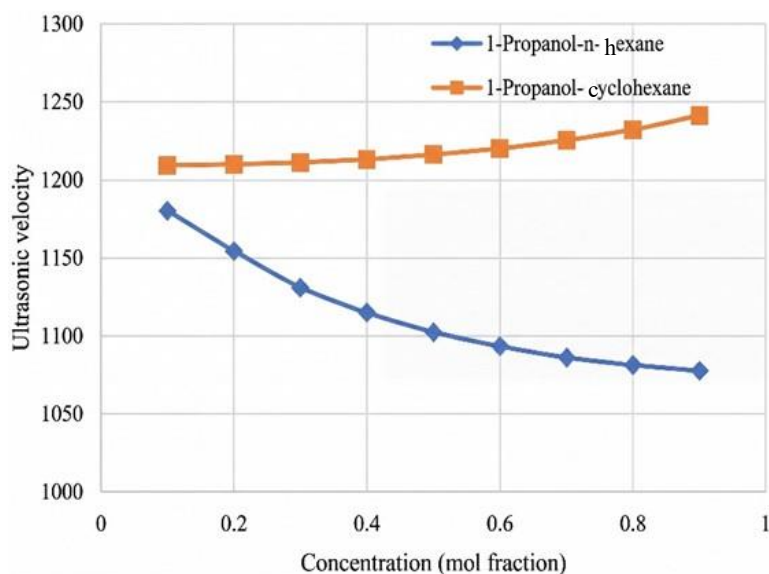


Figure 3. Ultrasonic velocity vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

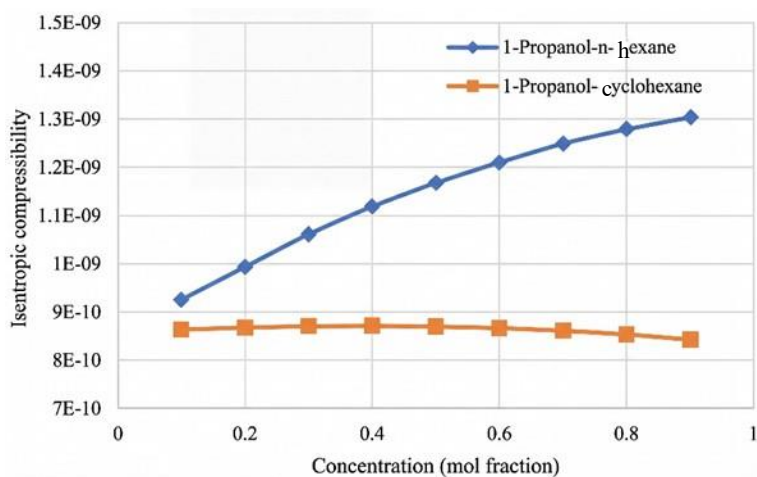


Figure 4. Isentropic compressibility vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

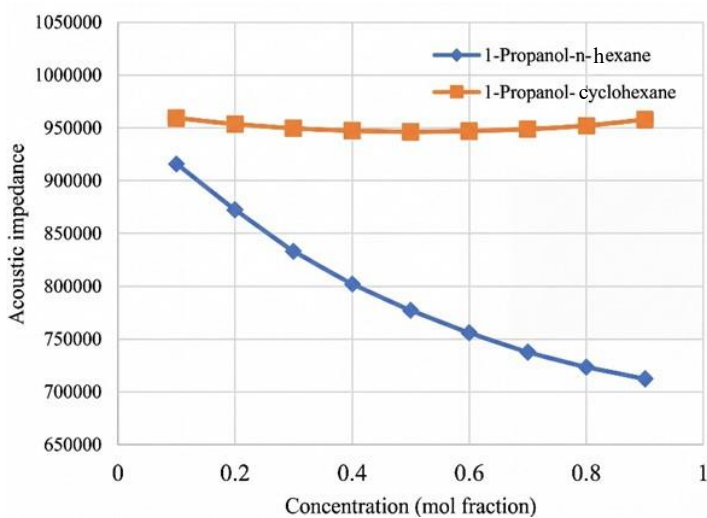


Figure 5. Acoustic impedance vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

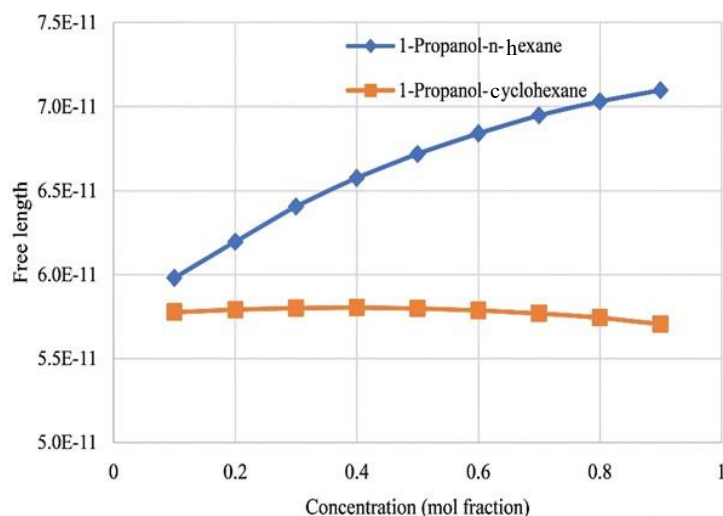


Figure 6. Free length vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

These relationships are clearly reflected in the systems investigated. As shown in Figure 5, the acoustic impedance varies inversely with isentropic compressibility, while Figure 6 demonstrates that intermolecular free length follows the same concentration-dependent trend as compressibility for the two binary mixtures. The consistently lower compressibility and free length and correspondingly higher acoustic impedance observed in the 1-propanol-cyclohexane system confirm a more compact molecular packing relative to the 1-propanol-n-hexane system. This enhanced association arises from the cyclic structure of cyclohexane, which enables more efficient packing with 1-propanol than the linear n-hexane analogue [37–41].

Free volume represents the effective space within a liquid in which the center of a molecule can move while remaining under the influence of the surrounding intermolecular potential field. It is inversely related to internal pressure, and variations in free volume, therefore, provide a sensitive measure of molecular association in solution. A decrease in intermolecular interactions whether due to weaker cohesive forces or reduced solute-solvent affinity leads to increased free volume, reflecting looser packing of molecules within the medium.

In this context, free volume serves as a valuable parameter for assessing the strength of intermolecular forces, with higher values corresponding to weaker association and more open structural arrangements.

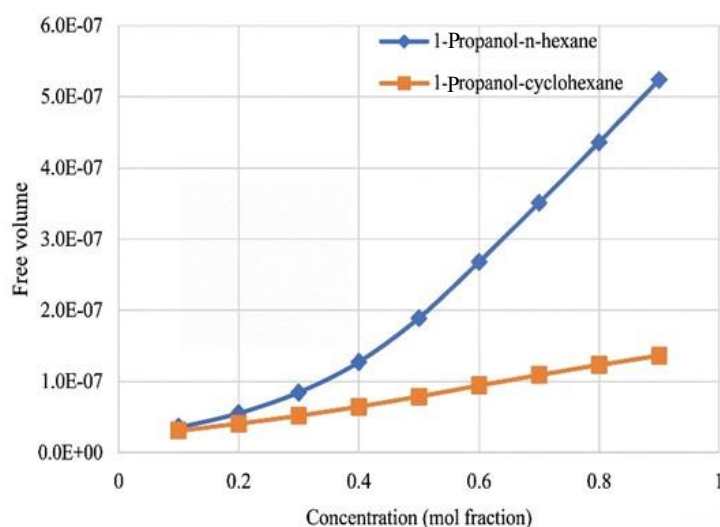


Figure 7. Free volume vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

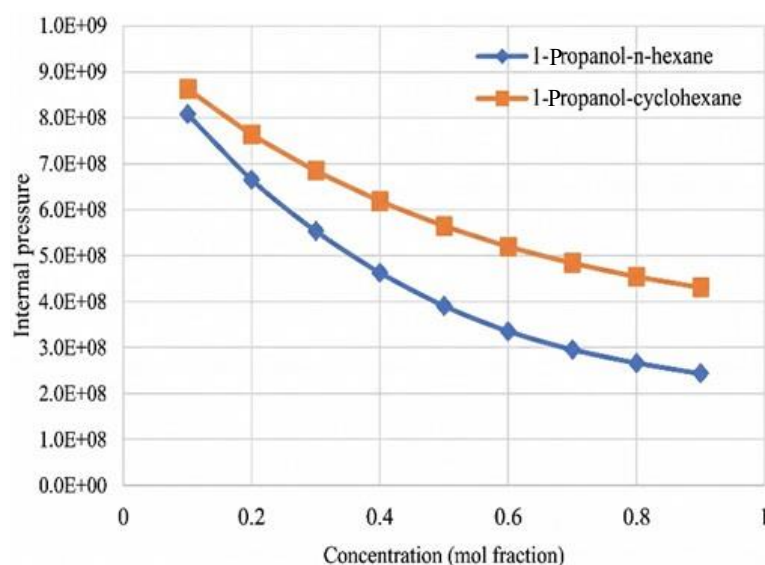


Figure 8. Internal pressure vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

The concentration-dependent behavior displayed in Figure 7 aligns with this interpretation. The free volume of the 1-propanol-n-hexane system is consistently greater than that of the 1-propanol-cyclohexane system, indicating a less compact molecular arrangement in the former. By contrast, the lower free volume observed for the 1-propanol-cyclohexane mixtures supports the conclusion, established from previous parameters, that the cyclic structure of cyclohexane promotes tighter packing and stronger molecular association than the linear n-hexane analogue [42–44].

Bulk properties of liquids are determined by the combined effects of intermolecular attractive and repulsive forces. While attractive forces dominate at moderate intermolecular distances, repulsive forces become significant only when molecules approach one another very closely. In liquids, molecular separations are larger than in solids, and the balance between these opposing forces establishes the effective cohesive environment within the bulk phase. This balance is expressed quantitatively as internal pressure.

Internal pressure reflects the net cohesive force resulting from all modes of molecular interaction, including solvent-solvent, solute-solvent, and solute-solute contributions. Because it responds sensitively to changes in intermolecular proximity and interaction strength, internal pressure is a valuable indicator of the microscopic structure and association within a liquid mixture.

The trend observed in Figure 8 supports this interpretation. The internal pressure of the 1-propanol-cyclohexane system is consistently higher than that of the corresponding 1-propanol-n-hexane mixtures. This enhancement can be attributed to stronger solute-solvent interactions and more efficient packing of molecules in the cyclohexane-containing solutions, facilitated by the compact cyclic geometry of cyclohexane relative to the extended structure of n-hexane. The slightly elevated internal pressure in the 1-propanol-cyclohexane system, therefore, substantiates the presence of stronger cohesive interactions within the mixture [12,45,46].

Relaxation time (τ) provides valuable insight into the degree of structural organization and packing within a liquid medium. In loosely packed systems, relaxation occurs rapidly because molecular equilibrium is disturbed and restored with minimal resistance. In contrast, closely packed media exhibit extended relaxation times, as molecular motion is constrained and disruption of equilibrium requires greater effort. Thus, an increase in relaxation time is indicative of enhanced molecular association within the system. Such close packing commonly arises from intermolecular interactions, such as hydrogen bonding, van der Waals forces, or dispersion forces. The greater the strength of these cohesive forces, the longer is the relaxation time. Relaxation time represents the interval required for excitation

energy introduced by an ultrasonic wave to convert into translational molecular motion. It is closely linked to the acoustic absorption coefficient, since absorption results from the finite delay between perturbation of molecules by the passing sound wave and their return to equilibrium.

The trend observed in Figure 9 supports this interpretation. The 1-propanol-cyclohexane system exhibits slightly longer relaxation times than the 1-propanol-n-hexane system. This behavior is consistent with a more closely packed structure in the cyclohexane-containing mixtures, further corroborating the stronger intermolecular interactions associated with the cyclic cyclohexane framework compared to the linear n-hexane analogue [28,47,48].

Ultrasonic absorption provides important insight into the physicochemical behavior of liquids and liquid mixtures, revealing information about composition, viscosity, molecular relaxation processes, and local microstructure. When an ultrasonic wave propagates through a medium, part of its mechanical energy is irreversibly lost, a phenomenon referred to as attenuation or classical absorption. Prior to the passage of ultrasound, the liquid exists as a homogeneous continuum however, interaction with the wave perturbs the medium and generates a transiently dispersed state. The observed absorption is, therefore, a composite effect arising from intrinsic, thermal, visco-inertial, and scattering contributions.

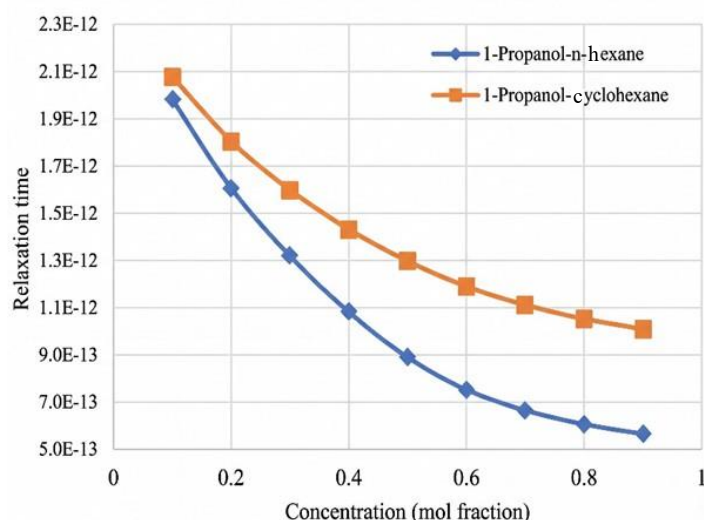


Figure 9. Relaxation time vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

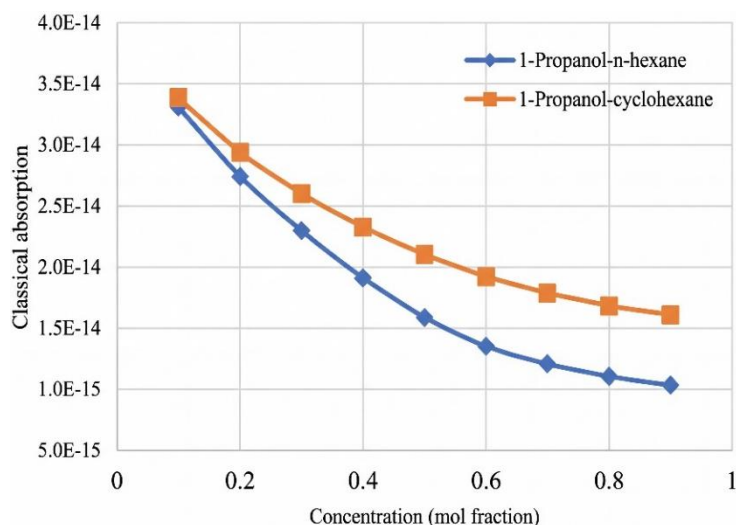


Figure 10. Classical absorption vs. n-hexane and cyclohexane concentration in 1-propanol at 298.15 K.

Intrinsic absorption represents direct conversion of acoustic energy into heat through interaction with the molecules of both the continuous and dispersed phases. Thermal absorption originates from temperature gradients established as the wave compresses and rarefies the medium, while visco-inertial losses arise from the resistance encountered when neighboring fluid layers slide past one another, particularly when density differences exist between transiently formed microdomains. A further contribution, often significant in structured or associating liquids, derives from molecular relaxation processes, whereby part of the ultrasonic energy is stored temporarily in perturbed molecular configurations before being released as heat.

The experimental behavior depicted in Figure 10 is consistent with these mechanistic considerations. The 1-propanol-cyclohexane system exhibits higher classical absorption than the corresponding 1-propanol-n-hexane mixtures across the composition range. This enhanced attenuation reflects stronger intermolecular association and more pronounced structural organization in the cyclohexane-containing solutions. The compact cyclic geometry of cyclohexane promotes closer packing and greater cohesive interactions with 1-propanol, which increases internal friction, restricts rapid molecular rearrangement, and intensifies both relaxation and visco-inertial contributions to energy loss. By contrast, the looser packing and weaker interactions in the 1-propanol-n-hexane system reduce resistance to acoustic propagation, leading to lower absorption. Thus, the attenuation trends observed in Figure 10 provide additional support consistent with velocity, compressibility, free length, internal pressure, and relaxation time data that molecular association is more pronounced in the 1-propanol-cyclohexane system than in the 1-propanol-n-hexane system [28,29].

CONCLUSION

The ultrasonic, acoustic, and viscosity studies of the binary systems 1-propanol-cyclohexane and 1-propanol-n-hexane provide clear and consistent evidence regarding the nature and extent of molecular interactions between the constituent components. Across all measured properties including ultrasonic velocity, isentropic compressibility, intermolecular free length, acoustic impedance, internal pressure, relaxation time, classical absorption, and viscosity a coherent trend emerges. The 1-propanol-cyclohexane mixtures exhibit higher ultrasonic velocity, viscosity, acoustic impedance, internal pressure, relaxation time, and classical absorption, accompanied by lower isentropic compressibility and intermolecular free length relative to the 1-propanol-n-hexane system.

These variations reflect enhanced molecular association and more efficient packing within the 1-propanol-cyclohexane mixtures, arising from the compact geometry and stronger cohesive tendencies of cyclohexane compared to the linear n-hexane analogue. The resulting interactions are attributed primarily to hydrogen bonding, van der Waals forces, and dispersion contributions, which collectively restrict molecular freedom and intensify energy dissipation under acoustic perturbation.

Taken together, the data confirms that cyclohexane forms a more structured and tightly bound mixed environment with 1-propanol than does n-hexane. This work, therefore, demonstrates the sensitivity of ultrasonic and thermodynamic parameters in characterizing solute-solvent interactions and provides a reliable framework for probing microstructural organization in mixed liquid systems.

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