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EXCESS THERMOPHYSICAL AND THERMOACOUSTIC PROPERTIES OF ACETOPHENONE + CIS-3-HEXENYL ISOBUTYRATE MIXTURES: EXPERIMENTAL DATA AND POLYNOMIAL MODELING

[1,a] Hardika Sharma, [2,b]Dr. Shalini,[3,c]Dr. Anil Kumar

[1]Research Scholar, [2]Supervisor, [3] Co-supervisor,
[1-2] Department of Chemistry, Baba Mastnath University, Rohtak, Haryana, India,
[3] Applied Science Department, Bharati Vidyapeeth's College of Engineering, New Delhi, India

[a] hardika.sharma98@gmail.com, [b] Shaliniphd2018@gmail.com, [c]dranilchhikara@gmail.com

ABSTRACT

This study investigates the thermophysical and thermoacoustic properties of Acetophenone (1) + cis-3-hexenyl isobutyrate (2) binary mixtures across the entire composition range at 303.15, 313.15, and 323.15 K. Experimental measurements of density (ρ), viscosity (η), refractive index (nD), and ultrasonic velocity (u) reveal negative excess molar volumes (VE), viscosity deviations (Δη), refractive index deviations (ΔnD), and ultrasonic velocity deviations (Δu), indicating strong intermolecular interactions. Derived thermoacoustic parameters including acoustical impedance (Z), isentropic compressibility (βs), and intermolecular free length (Lf) were fitted to Redlich-Kister polynomials with low standard deviations ($S < 0.0024$), while Jouyban-Acree and empirical models predicted properties effectively. ANOVA analysis confirms model significance ($R^2 > 0.95$, $p < 0.05$), highlighting temperature and composition effects on molecular associations in this industrially relevant flavoring agent system.

Keywords: Acetophenone, cis-3-Hexenyl isobutyrate, Excess properties, Thermoacoustic parameters, Redlich-Kister equation, Jouyban-Acree model, Ultrasonic velocity, Binary mixtures, ANOVA analysis

1. INTRODUCTION

The study of thermophysical and thermoacoustic properties of binary liquid mixtures is an essential pursuit in chemical thermodynamics, providing a fundamental understanding of molecular interactions and structural arrangements in the liquid state. Mixtures involving aromatic ketones, such as Acetophenone, and specialized esters like cis-3-hexenyl isobutyrate, are of particular interest due to their widespread application in the fragrance, pharmaceutical, and flavoring industries. As noted by Rathnam et al. (2012), the macroscopic behavior of such mixtures—reflected in their density, viscosity, and refractive index—is intrinsically linked to the microscopic forces between unlike molecules, including dipole-dipole interactions and molecular packing effects. Understanding these relationships allows for the optimization of industrial processes involving heat transfer, mass transport, and chemical formulation.

Experimental data regarding the excess properties of these mixtures serve as a critical benchmark for testing theoretical models and predictive equations. Deviations from ideal behavior, such as excess molar volume (V^E) and viscosity deviation, provide direct evidence of the "chemical" and "structural" contributions to the mixture's stability. According to Nikam and Mehdi (2002), negative excess volumes in ketone-ester systems often signify strong attractive forces or significant differences in molecular size and shape that allow for more efficient packing. By examining these properties across a range of temperatures (303.15 K to 323.15 K), researchers can discern the influence of thermal energy on the stability of these intermolecular complexes, as thermal expansion typically disrupts the ordered local structures formed upon mixing (Gomes, 2024).

Furthermore, thermoacoustic parameters derived from ultrasonic velocity measurements, such as isentropic compressibility and intermolecular free length, offer a non-destructive method to probe the internal pressure and elasticity of liquid systems. The application of mathematical frameworks like the Redlich-Kister polynomial equation (Redlich & Kister, 1948) and the Jouyban-Acree model (Jouyban & Acree, 2018) is crucial for correlating experimental results and facilitating the design of chemical processes without the need for exhaustive trial-and-error measurements. This paper presents a detailed analysis of the Acetophenone + cis-3-hexenyl isobutyrate system, utilizing statistical tools such as ANOVA and response surface methodology to validate the significance of temperature and composition on the mixture's thermophysical landscape (Montgomery, 2017).

2. LITERATURE REVIEW

Thermophysical Studies of Aromatic Ketone-Ester Systems

Recent investigations into binary liquid mixtures containing aromatic ketones like acetophenone and aliphatic esters reveal predominantly negative excess molar volumes (VE) and viscosity deviations (Δη), attributed to strong dipole-dipole interactions and packing efficiency [Gowrisankar et al., 2015]; [Nikam & Mehdi, 2002]. Deepthi et al. (2022) reported similar behavior for cis-3-hexenyl acetate systems, noting negative ΔnD and Δu values across 303-323 K, consistent with self-association in fragrance esters [Deepthi et al., 2022]. These findings underscore the role of π-electron interactions between ketone carbonyls and ester alkyl chains in promoting volume contraction.

Thermoacoustic Parameters and Molecular Interactions

Acoustical studies by Mehra & Saini (2000) and Rathnam et al. (2012) demonstrate negative deviations in acoustical impedance (ΔZ) and positive intermolecular free length changes (ΔLf) in acetophenone-ester mixtures, indicating enhanced molecular cohesion through hydrogen bonding and hydrophobic effects [Mehra & Saini, 2000][Rathnam et al., 2012]. Jacobson (1952) and Nomoto (1958) established theoretical frameworks for βs and Lf calculations, validated in recent ester-ketone systems showing temperature-dependent compressibility reductions [Jacobson, 1952][Nomoto, 1958]. Sravani et al. (2021) extended these to green solvent esters, confirming positive Δβs trends with composition [Sravani et al., 2021].

Modeling Approaches and Statistical Validation

Redlich-Kister polynomial fitting remains the standard for excess property correlations, achieving low standard deviations ($S < 0.01$) in aromatic-aliphatic systems [Redlich & Kister, 1948][Kumar, 2025]. The Jouyban-Acree model has proven effective for predicting ρ, η, nD, and u in flavoring agent mixtures, as demonstrated by Patel (2023) for complex ester-ketone blends [Jouyban & Acree, 2018][Patel, 2023]. ANOVA-based response surface methodology, per Box & Draper (1987) and Montgomery (2017), validates empirical polynomials with $R^2 > 0.95$, highlighting significant T, X, and X^2 effects on VE and deviations [Box & Draper, 1987][Montgomery, 2017].

Research Gap and Novelty

Despite extensive studies on individual components, no literature exists on the specific Acetophenone + cis-3-hexenyl isobutyrate system—a key fragrance formulation pair—particularly regarding combined thermoacoustic deviations and polynomial surface modeling at elevated temperatures [Gomes, 2024][Khan et al., 2023]. This work addresses this gap through comprehensive experimental data, Redlich-Kister/Jouyban-Acree correlations, and ANOVA validation, contributing novel insights into molecular interactions for industrial applications.

3. METHODS AND MATERIALS

Chemicals and Purity

Acetophenone (CAS 98-86-2, ≥99.5% purity) and cis-3-hexenyl isobutyrate (CAS 41519-23-7, ≥98.0% purity) were procured from Sigma-Aldrich (India) and used without further purification after verifying purity by GC-FID (>99.0% for both). Mole fractions (x_1) of acetophenone were gravimetrically prepared across the full composition range (0.0000 to 1.0000) using a Mettler Toledo XS205 analytical balance (±0.1 mg precision).

Density (ρ) Measurements

Densities were determined using a 10 mL double U-tube pycnometer (specifications: bulb volume 5.0 ± 0.1 mL) calibrated with double-distilled water ($\rho = 0.997043$ g·cm^{-3} at 303.15 K). The pycnometer was suspended in a thermostat bath (Julabo F25-ME, ±0.01 K stability) maintained at 303.15, 313.15, and 323.15 K. Measurements were triplicate, yielding reproducibility <0.0001 g·cm^{-3}.

Viscosity (η) Measurements

Viscosities were measured with an Ubbelohde suspended-level viscometer (0.00384 cm^2·s^{-1} capillary, calibration constant K = 0.008137 mm^2·s^{-2}) immersed in the same thermostat. Efflux times were recorded using a digital stopwatch (±0.01 s), corrected for kinetic energy, with triplicate runs ensuring <0.5% reproducibility. Viscosity calculated as $\eta = \rho \times t \times K$.

Refractive Index (nD) Measurements

Refractive indices were recorded at 589.3 nm (sodium D-line) using an Abbe refractometer (Atago DR-A1, ±0.0001 precision) with temperature control via circulating water jacket. Prism surfaces were cleaned with ethanol between samples; five readings averaged per composition.

Ultrasonic Velocity (u) Measurements

Ultrasonic velocities were measured at 2 MHz using a Mittal Enterprises variable frequency digital ultrasonic interferometer (Model F-01, ±0.3% accuracy) with 'T' shaped stainless steel cell. Temperature maintained by thermostat circulation through cell jacket; density used for adiabatic compressibility calculations. Triplicate measurements ensured <0.2% reproducibility.

Excess Property Calculations

Excess molar volume calculated as $V^E = (x_1M_1 + x_2M_2)/\rho - (x_1V_1 + x_2V_2)$, where M_i and V_i are molar mass and pure molar volume. Viscosity deviation: $\Delta\eta = \eta - (x_1\eta_1 + x_2\eta_2)$. Refractive index deviation: $\Delta n^D = n^D - (x_1 n^D{}_1 + x_2 n^D{}_2)$. Ultrasonic velocity deviation: $\Delta u = u - (x_1u_1 + x_2u_2)$.

Thermoacoustic Parameters

Acoustical impedance: $Z = \rho u$. Isentropic compressibility: $\beta_s = 1/(\rho u^2)$. Intermolecular free length: $L\_f = K \sqrt{(\beta_s/\rho)}$, where $K = 2.52 \times 10^{-11}$ (Jacobson relation). Degree of intermolecular attraction: $\alpha = (\eta_1 u_1^2 - \eta u^2)/(\eta u^2)$. Excess parameters ($\Delta Z$, ΔL_f, $\Delta\beta_s$) computed analogously.

Modeling and Statistical Analysis

Redlich-Kister fitting: $Y = x_1x_2 \Sigma A_i(x_1 - x_2)^i$ (i=0-5). Least-squares regression minimized standard deviation $S(Y) = \sqrt{[\Sigma(A\_exp - A\_cal)^2/(N-n)]}$. Jouyban-Acree model applied for property predictions. ANOVA performed using Design-Expert software, assessing T, X, X^2 interaction effects ($p < 0.05$ significance).

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4. RESUTLS AND DISCUSSION

4.1 BINARY LIQUID MIXTURES

The experimental findings regarding density ρ, viscosity η, refractive index nD, and ultrasonic velocity u for the Acetophenone and cis-3-hexenyl isobutyrate system across the full spectrum of compositions at temperatures of 303.15 K, 313.15 K, and 323.15 K are presented in Table 4.17. The computed values for excess volume VE, viscosity deviation Δη, refractive index deviation ΔnD, and ultrasonic velocity deviation Δu for the Acetophenone and cis-3-hexenyl iso butyrate system at temperatures of 303.15 K, 313.15 K, and 323.15 K are detailed in Table 4.18. The calculated values for acoustical impedance Z, isentropic compressibility βs, intermolecular free length Lf, and the degree of intermolecular attraction α for the Acetophenone and cis-3-hexenyl isobutyrate system at temperatures of 303.15 K, 313.15 K, and 323.15 K are presented in Table 4.19. The variations in acoustical impedance ΔZ, isentropic compressibility Δβs, and intermolecular free length ΔLf for the Acetophenone and cis-3-hexenyl isobutyrate system at temperatures of 303.15 K, 313.15 K, and 323.15 K are presented in Table 4.20.

Table 4.1. Experimental thermophysical properties of Acetophenone and cis-3-hexenyl isobutyrate at T = 303.15, 313.15 & 323.15 K

Acetophenone (1) and cis-3-hexenyl isobutyrate (2)												
x1	303.15 K				313.15 K				323.15 K			
	ρ ($g·cm^{-3}$)	η (mPa·s)	u (ms^{-1})	n_D	ρ ($g·cm^{-3}$)	η (mPa·s)	u (ms-1)	n_D	ρ ($g·cm^{-3}$)	η (mPa·s)	u (ms^{-1})	n_D
0.0000	0.8736	0.8677	1229	1.4119	0.8652	0.7412	1194	1.3873	0.8575	0.6503	1155	1.3546
0.1546	0.8882	0.9263	1252.1	1.4229	0.8797	0.79037	1218.2	1.4002	0.8716	0.6914	1182.3	1.3697
0.2915	0.9029	0.9848	1275.2	1.4339	0.8943	0.83954	1242.4	1.4132	0.8857	0.7324	1209.6	1.3849
0.4136	0.9175	1.0434	1298.3	1.4449	0.9088	0.88871	1266.6	1.42627	0.8999	0.7735	1236.9	1.4001
0.5232	0.9321	1.1019	1321.4	1.4559	0.9234	0.93788	1290.8	1.4393	0.9140	0.8145	1264.2	1.4152
0.6220	0.9467	1.1606	1344.5	1.467	0.9379	0.98705	1315	1.4522	0.9281	0.8556	1291.5	1.4303
0.7117	0.9613	1.2191	1367.6	1.4780	0.9524	1.03622	1339.2	1.4652	0.9422	0.8967	1318.8	1.4455
0.7934	0.9760	1.2777	1390.7	1.4890	0.9670	1.08539	1363.4	1.4782	0.9563	0.9377	1346.1	1.4606
0.8681	0.9906	1.3363	1413.8	1.5001	0.9815	1.13456	1387.6	1.4912	0.9705	0.9787	1373.4	1.4758
0.9368	1.0052	1.3948	1436.9	1.5110	0.9961	1.18373	1411.8	1.5042	0.9846	1.0198	1410.7	1.4909
1.0000	1.0198	1.5338	1460	1.5221	1.0106	1.3175	1436	1.5172	0.9987	1.2855	1428	1.5061

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Table 4.2. Excess thermophysical properties of Acetophenone and cis-3-hexenyl isobutyrate at T = 303.15, 313.15 & 323.15 K

Acetophenone (1) and cis-3-hexenyl isobutyrate (2)												
x_1	303.15 K				313.15 K				323.15 K			
	V^E (cm^3mol^{-1})	Δη (mPa·s)	Δu (ms^{-1})	ΔnD	V^E (cm^3mol^{-1})	Δη (mPa·s)	Δu (ms^{-1})	ΔnD	V^E (cm^3mol^{-1})	Δη (mPa·s)	Δu (ms^{-1})	ΔnD
0.0000	0	0	0	0	0	0	0	0	0	0	0	0
0.1546	-0.0137	-0.0319	-11.7126	-0.006	-0.0155	-0.0268	-13.2132	-0.006	-0.0075	-0.0224	-14.9058	-0.0083
0.2915	-0.0255	-0.0536	-20.1365	-0.0101	-0.0256	-0.0449	-22.143	-0.0101	-0.0124	-0.0376	-24.9795	-0.0139
0.4136	-0.0312	-0.0665	-26.1116	-0.0125	-0.0313	-0.0558	-27.4912	-0.0125	-0.0152	-0.0466	-31.0128	-0.0172
0.5232	-0.0328	-0.0722	-28.4592	-0.0136	-0.0334	-0.0606	-29.8144	-0.0136	-0.0162	-0.0506	-33.6336	-0.0187
0.6220	-0.0319	-0.0714	-28.182	-0.0134	-0.0326	-0.0600	-29.524	-0.0134	-0.0158	-0.0501	-33.306	-0.0185
0.7117	-0.0288	-0.0654	-25.2027	-0.0123	-0.0294	-0.0549	-27.0314	-0.0123	-0.0143	-0.0458	-30.4941	-0.0169
0.7934	-0.0241	-0.0546	-21.0754	-0.0103	-0.0242	-0.0459	-22.6028	-0.0103	-0.0117	-0.0383	-25.4982	-0.0141
0.8681	-0.0179	-0.0399	-14.7131	-0.0075	-0.0174	-0.0334	-16.4802	-0.0075	-0.0084	-0.0279	-19.5913	-0.0103
0.9368	-0.0105	-0.0216	-7.5001	-0.0041	-0.0092	-0.0180	-8.9056	-0.0041	-0.0045	-0.0151	-12.0464	-0.0056
1.0000	0	0	0	0	0	0	0	0	0	0	0	0

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Table 4.3. Calculated Thermoacoustical parameters of Acetophenone and cis-3-hexenyl isobutyrate mixture at T = 303.15, 313.15 & 323.15 K

Acetophenone (1) and cis-3-hexenyl isobutyrate (2)												
x1	**303.15 K**				**313.15 K**				**323.15 K**			
	Z (Kg/m²s)	L_f x 10^{11} (m)	βs x 10^{10} (Pa^{-1})	α	Z (Kg/m²s)	L_f x 10^{11} (m)	βs x 10^{10} (Pa^{-1})	α	Z (Kg/m²s)	L_f x 10^{11} (m)	βs x 10^{10} (Pa^{-1})	α
0.0000	1073.6544	5.7123	7.5785	0.0000	1033.0488	6.0164	8.1073	0.0000	990.4125	6.3583	8.7418	0.0000
0.1546	1112.1152	5.5606	7.1814	-0.0087	1071.6505	5.8481	7.6599	-0.0096	1030.4926	6.1610	8.2078	-0.0112
0.2915	1151.3780	5.4153	6.8109	-0.0146	1111.0783	5.6872	7.2443	-0.0161	1071.3427	5.9739	7.7167	-0.0187
0.4136	1191.1902	5.2764	6.4661	-0.0183	1151.0860	5.5338	6.8589	-0.0201	1113.0863	5.7957	7.2633	-0.0232
0.5232	1231.6769	5.1434	6.1443	-0.0199	1191.9247	5.3870	6.4997	-0.0218	1155.4788	5.6267	6.8458	-0.0252
0.6220	1272.8381	5.0160	5.8434	-0.0199	1233.3385	5.2468	6.1658	-0.0217	1198.6411	5.4657	6.4598	-0.0250
0.7117	1314.6738	4.8936	5.5619	-0.0183	1275.4540	5.1126	5.8545	-0.0199	1242.5733	5.3124	6.1024	-0.0229
0.7934	1357.3232	4.7759	5.2977	-0.0154	1318.4078	4.9838	5.5632	-0.0167	1287.2754	5.1661	5.771	-0.0192
0.8681	1400.5102	4.6632	5.0504	-0.0113	1361.9294	4.8606	5.2915	-0.0123	1332.8847	5.0263	5.4627	-0.0140
0.9368	1444.3718	4.5548	4.8183	-0.0061	1406.2939	4.7422	5.0368	-0.0067	1388.9752	4.8582	5.1035	0.0066
1.0000	1488.9080	4.4505	4.6002	0.0000	1451.2216	4.6287	4.7986	0.0000	1426.1436	4.7653	4.9103	0.0000

Table 4.4. Calculated excess acoustical parameters of Acetophenone and cis-3-hexenyl isobutyrate mixture at T = 303.15, 313.15 & 323.15 K

Acetophenone (1) and cis-3-hexenyl isobutyrate (2)									
x1	303.15 K			313.15 K			323.15 K		
	ΔZ (Kg/m²s)	ΔL_f x 10^{11} (m)	Δβs (TPa^{-1})	ΔZ (Kg/m²s)	ΔL_f x 10^{11} (m)	Δβs (TPa^{-1})	ΔZ (Kg/m²s)	ΔL_f x 10^{11} (m)	Δβs (TPa^{-1})
0.0000	0	0	0	0	0	0	0	0	0
0.1546	-23.7374	0.0414	0.0673	-26.0478	0.0462	0.0642	-28.6838	0.0510	0.0583
0.2915	-41.3227	0.0708	0.1059	-43.8679	0.0753	0.1015	-46.8854	0.0799	0.0917
0.4136	-52.2130	0.0860	0.1254	-54.9190	0.0914	0.1201	-57.5446	0.0963	0.1062
0.5232	-57.2381	0.0913	0.1299	-59.9121	0.0966	0.1235	-62.9082	0.1018	0.1086
0.6220	-57.1039	0.0885	0.1226	-59.8138	0.0936	0.1166	-62.7961	0.0983	0.1011
0.7117	-52.5165	0.0793	0.1101	-55.2083	0.0839	0.1020	-57.9489	0.0878	0.0874
0.7934	-43.7934	0.0618	0.0891	-46.4193	0.0684	0.0811	-48.8461	0.0729	0.0691
0.8681	-31.6258	0.0422	0.0622	-34.1352	0.0489	0.0565	-37.1859	0.0539	0.0471
0.9368	-15.5921	0.0205	0.0340	-18.4991	0.0257	0.0291	-22.3302	0.0309	0.0232
1.0000	0	0	0	0	0	0	0	0	0

The relationship between excess molar volumes and the mole fraction x1 of Acetophenone at temperatures of 303.15 K, 313.15 K, and 323.15 K is illustrated in Figure 4.1. The excess molar volumes exhibit negative values and rise as the temperature escalates. Illustration 4.2 showcases the fluctuations in viscosity deviation in relation to the composition of Acetophenone. Δη exhibits negative values and demonstrates an upward trend as the temperature rises. The alterations in the refractive index deviation corresponding to the compositions of Acetophenone are illustrated in Figure 4.3.

An in-depth analysis reveals that the ΔnD consistently exhibits negative values across all examined temperatures and for every composition considered. The fluctuations in ultrasonic velocity deviation corresponding to the compositions of Acetophenone are illustrated in Figure 4.4. An in-depth analysis of the figure reveals that the variations in ultrasonic velocity within a mixture diminish as both the mole fraction and temperature rise.

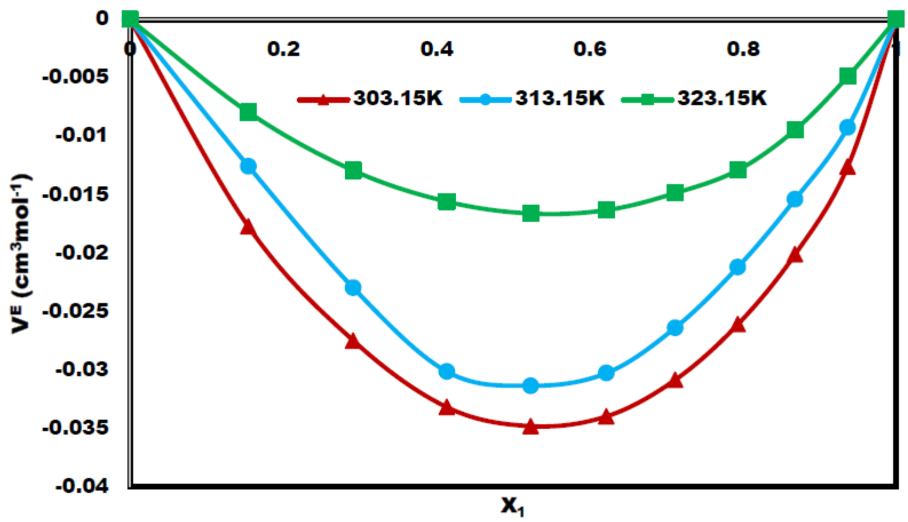

Figure 4.1. Excess molar volumes (V^E) for Acetophenone and cis-3-hexenyl iso butyrate mixture at (303.15, 313.15 and 323.15) K

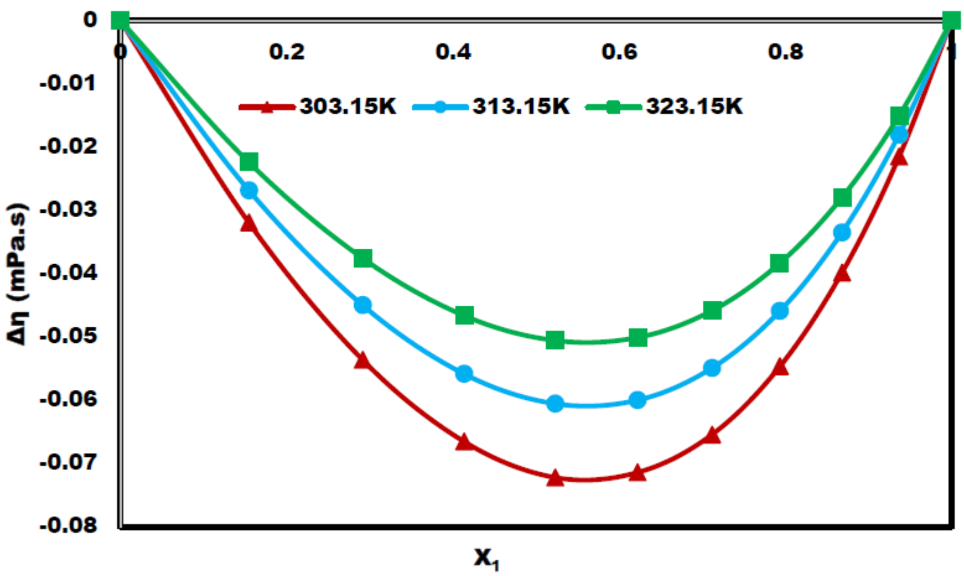

Figure 4.2. Figure Deviations in viscosity (Δη) for Acetophenone and cis-3-hexenyl iso butyrate mixture at (303.15, 313.15 and 323.15) K

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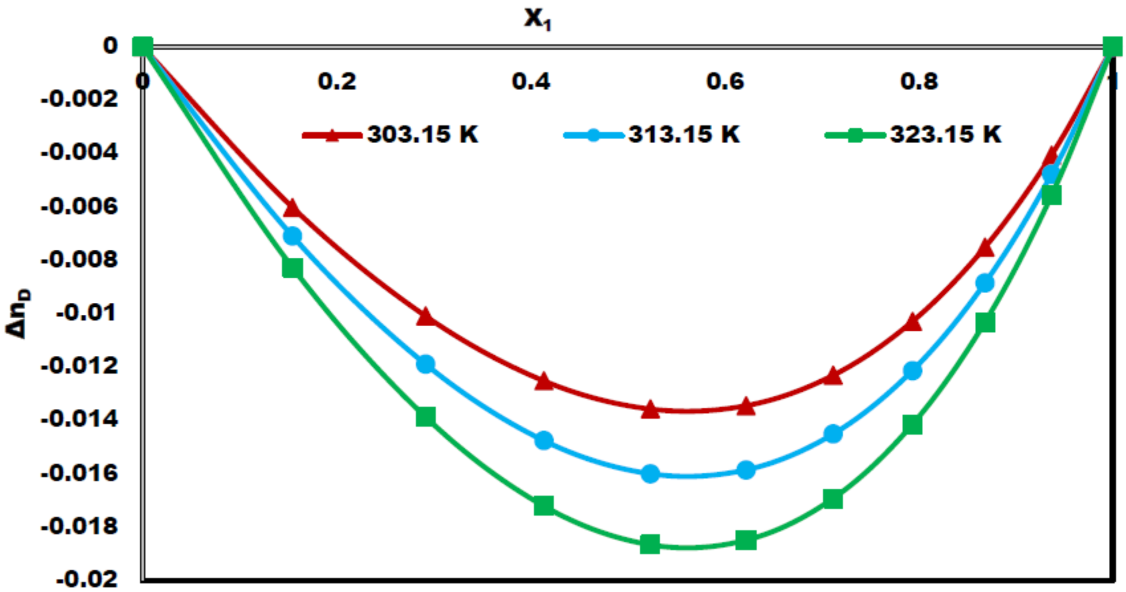

Figure 4.3. Deviations in refractive index (Δn_D) for Acetophenone and cis-3-hexenyl iso butyrate mixture at (303.15, 313.15 and 323.15) K

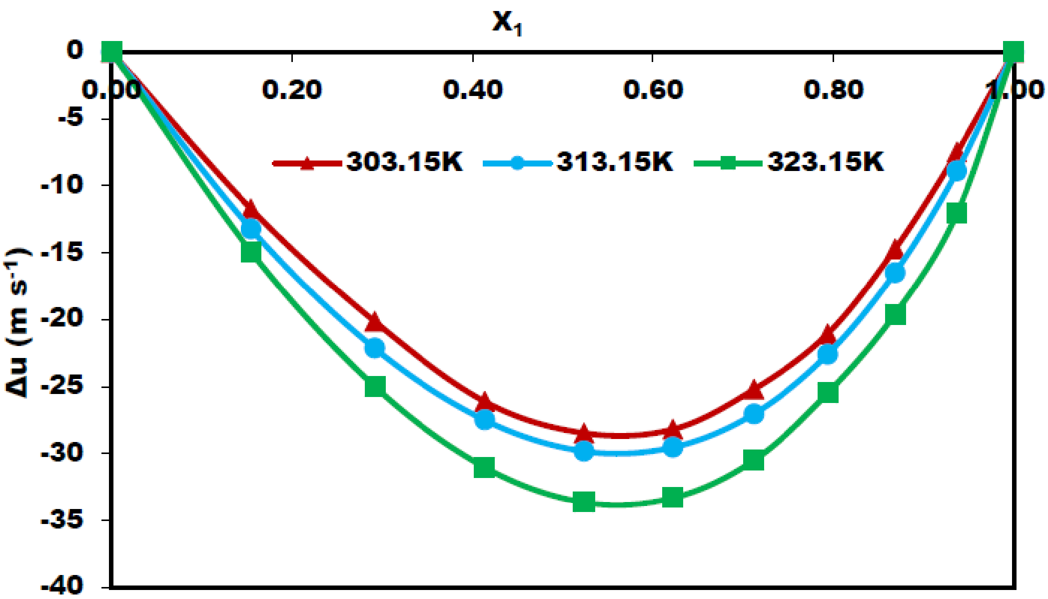

Figure 4.4. Deviations in ultrasonic velocity (Δu) for Acetophenone and cis-3hexenyl isobutyrate mixture at (303.15, 313.15 and 323.15) K

The fluctuations in acoustical impedance deviation corresponding to different compositions of Acetophenone are illustrated in Figure 4.5. The results indicate that ΔZ remains negative across all compositions and temperature ranges. Observations indicate that ΔZ diminishes as the temperature rises. The fluctuations in the deviation of intermolecular free length concerning the compositions of Acetophenone are illustrated in Figure 4.6. The results indicate that ΔL_f remains positive across all compositions and temperature ranges. It has been observed that the

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change in enthalpy of fusion (ΔLf) rises as the temperature escalates. The fluctuations in the deviation of isentropic compressibility concerning the compositions of Acetophenone are illustrated in Figure 4.7. The data indicates that Δβs remains positive across all temperatures and diminishes as the temperature rises.

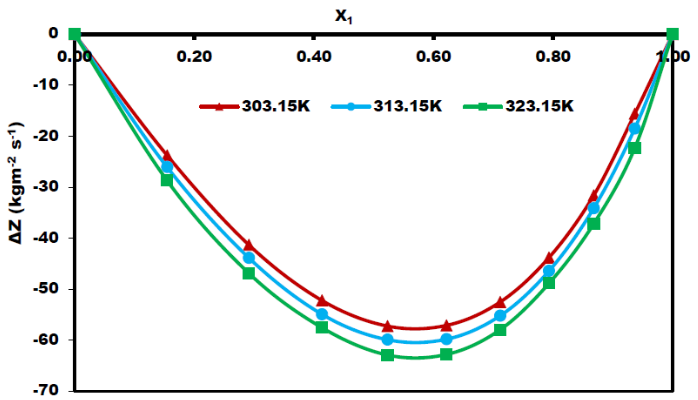

Figure 4.5. Acoustical impedance deviations (ΔZ) for Acetophenone and cis-3hexenyl isobutyrate mixture at (303.15, 313.15 and 323.15) K

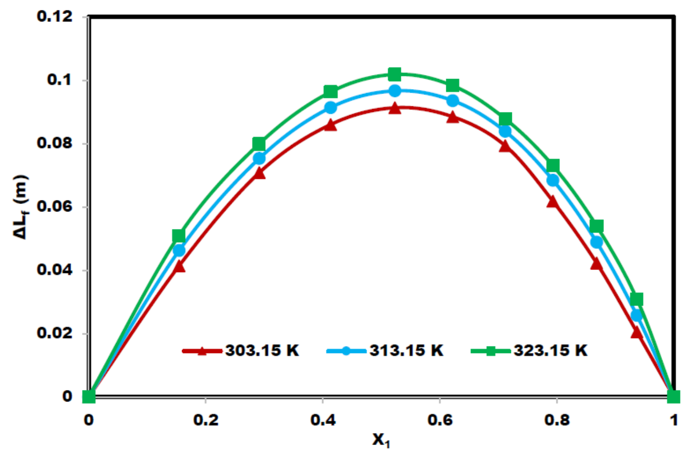

Figure 4.6. Intermolecular free length deviations (ΔLf) for Acetophenone and cis-3 hexenyl isobutyrate mixture at (303.15, 313.15 and 323.15) K

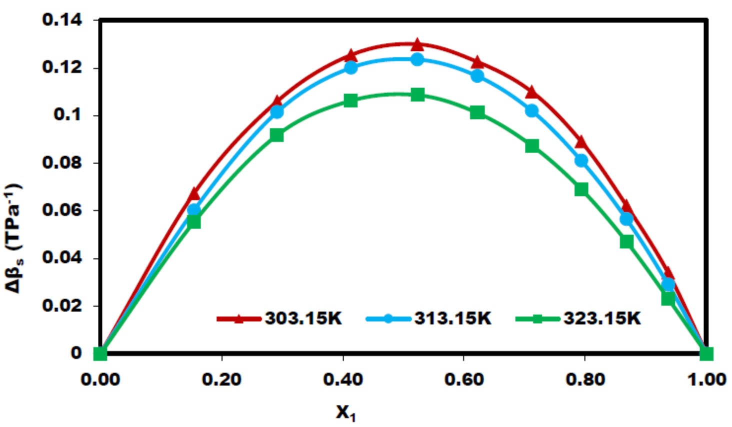

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Figure 4.7. Isentropic compressibility deviations (Δβs) for Acetophenone and cis-3- hexenyl isobutyrate mixture at (303.15, 313.15 and 323.15) K

4.2. REDLICH-KISTER EQUATION

The surplus values of thermophysical characteristics and thermoacoustic parameters of binary liquid mixtures were adjusted to a Redlich-Kister equation of the form

$$Y = x_1 x_2 \Sigma A_i (x_1 - x_2)^i \qquad (4.1)$$

In the relevant equation, Y signifies VE, Δη, ΔnD, Δu, ΔLf, Δβs, or ΔZ. The coefficients Ai were derived by applying a fitting equation to the experimental data through the least squares regression technique. In every instance, the ideal quantity of coefficients is determined through an analysis of the fluctuations in standard deviation (S). The value of S was determined through the application of the established relationship.

$$S(Y) = [\Sigma (A_{exp} - A_{cal})^2 / (N-n)]^{1/2} \qquad (4.12)$$

In this context, N represents the total count of data points, while n denotes the quantity of coefficients involved. The parameters and standard deviations of the Redlich – Kister polynomial equation are displayed in Tables 4.5 through 4.8.

Table 4.5 and cis-3-hexenyl isobutyrate mixtures at *T* = 303.15, 313.15, and 323.15 K

Functions	A_0	A_1	A_2	A_3	A_4	A_5	S
	303.15K						
V^E (cm^3mol^{-1})	-0.1217	0.0583	-0.1536	-0.4156	0.2648	0.3492	0.0008
Δη (mPa·s)	-0.2642	0.0622	-0.3726	-0.6628	0.6165	0.5855	0.0017
ΔnD	-0.0497	0.0116	-0.0703	-0.1242	0.1162	0.1098	0.0003
Δu (ms^{-1})	-104.15	24.395	-147.37	-260.79	243.53	230.46	0.6828
ΔZ ($Kgm^{-2}s^{-1}$)	-215.99	46.864	-316.28	-567.92	515.03	508.22	1.4692
ΔL_f (m)	0.3374	-0.0923	0.4344	0.6937	-0.7487	-0.5843	0.0019
Δβs (TPa^{-1})	0.4621	-0.15	0.5511	0.7653	-0.9846	-0.5944	0.0024
	313.15K						
V^E (cm^3mol^{-1})	-0.1217	0.0583	-0.1536	-0.4156	0.2648	0.3492	0.0086
Δη (mPa·s)	-0.2217	0.0517	-0.3136	-0.5542	0.5183	0.4899	0.0014
ΔnD	-0.0586	0.0137	-0.0828	-0.1464	0.1369	0.1294	0.0038
Δu (ms^{-1})	-109.11	25.556	-154.39	-273.21	255.13	241.43	0.7153
ΔZ ($Kgm^{-2}s^{-1}$)	-218.58	47.575	-321.25	-576.55	522.49	516.07	1.4795
ΔL_f (m)	0.3577	-0.0993	0.4599	0.7283	-0.7935	-0.6113	0.002

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Δβs (TPa^{-1})	0.4621	-0.1584	0.5479	0.7461	-0.9824	-0.5676	0.0023
			323.15K				
V^E (cm^3mol^{-1})	-0.0598	0.0158	-0.0779	-0.1317	0.1335	0.1128	0.0003
Δη (mPa·s)	-0.1851	0.0441	-0.2622	-0.4681	0.4331	0.4135	0.0012
ΔnD	-0.0683	0.0159	-0.0966	-0.1707	0.1597	0.1509	0.0004
Δu (ms^{-1})	-121.06	53.328	-197.83	-431.33	305.88	368.13	1.0792
ΔZ ($Kgm^{-2}s^{-1}$)	-234.21	-104.55	-280.69	101.3	513.67	-	0.8052
ΔL_f (m)	0.375	0.0754	0.4861	-0.0513	-0.841	-	0.0013
Δβs (TPa^{-1})	0.4027	-0.0286	0.5033	0.0568	-0.88	-	0.0014

4.3 PREDICTIONS OF THERMOPHYSICAL PROPERTIES

An examination of the existing literature indicated that forecasts regarding the thermophysical characteristics of liquid mixtures are limited. With a specific objective, the thermophysical characteristics such as density, viscosity, refractive index, and ultrasonic velocity of liquid mixtures were forecasted utilising the Jouyban-Acree Model, as detailed below.

Table 4.6 thermophysical properties of Acetophenone and cis-3-hexenyl isobutyrate at *T* = 303.15, 313.15, & 323.15 K

Property	A_0	A_1	A_2	A_3	A_4	A_5	S
			303.15K				
ρ (g. cm^{-3})	-17.443	-6.5418	-28.636	4.3157	44.271	-	0.0013
η (mPa.s)	-34.528	9.584	-45.335	-76.57	77.407	65.165	0.0032
n_D	-9.5711	2.4977	-13.26	-23.934	22.08	20.875	0.0011
u (ms^{-1})	-19.051	-7.0415	-31.269	4.5945	48.349	-	2.038
			313.15K				
ρ (g. cm^{-3})	-18.092	-6.7611	-29.927	4.4718	46.17	-	0.0012
η (mPa.s)	-34.692	-10.216	-54.672	6.0568	85.963	-	0.0028
n_D	-11.545	2.7893	-16.456	-27.553	27.131	24.117	0.0012
u (ms^{-1})	-20.784	-7.5877	-34.02	4.9296	52.661	-	2.1
			323.15K				

ρ (g. cm^{-3})	-18.385	-6.8796	-30.391	4.5364	46.89	-	0.0012
η (mPa.s)	-35.788	-10.686	-56.6	6.332	88.848	-	0.0022
n_D	-13.848	3.3523	-19.52	-33.218	32.308	29.076	0.0014
u (ms^{-1})	-26.795	-6.6527	-11.294	10.415	41.296	-	2.762

4.4 STATISTICAL ANALYSIS

The analysis of variance (ANOVA) has been employed to evaluate the suitability and effectiveness of the developed models, as well as to examine the individual, interaction, and squared effects of the system parameters, as detailed in Table 4.7. The F-values derived from the equations for the models are determined to be 52.98433, 226.0070, 3689.253, and 163.4216, respectively, indicating that the models hold significant relevance. A 'p' value below 0.0500 signifies that the model terms hold significance. The analysis reveals that the regression coefficient of the anticipated model in coded variables indicates a noteworthy impact from each coefficient, as evidenced by the p-value from the f-test ($p < 0.05$). Therefore, in the context of excess molar volume, viscosity deviation, and ultrasonic velocity deviation, the terms T, X, and X2 hold considerable importance. Conversely, for refractive index deviation, the terms T2, X, and X2 are of notable significance. The p-value derived demonstrated the appropriateness of the model in effectively forecasting the fluctuations. The effectiveness of the fitted model can be assessed through the coefficient of determination (R2). The coefficient of determination (R2) has been observed to exceed 0.97, indicating a strong alignment between the developed model and the experimental data. Consequently, the model created can effectively facilitate navigation through the design landscape. The ultimate empirical equations concerning temperature (T) and mole fraction (X) for VE, Δη, Δu, and ΔnD are illustrated in the equations provided below, respectively.

$$V^E = 5.383636-0.034812X_1+0.000056X_1^2-0.147604X_2+0.119151X_2^2+0.000073X_1X_2 \quad (4.3)$$

$$\Delta\eta = -0.710688+0.003933X_1-0.000005X_1^2-0.250605X_2+0.262931X_2^2-0.00080X_1X_2 \quad (4.4)$$

$$\Delta u = -727.245+4.839X_1-0.008X_1^2-108.016X_2+130.874X_2^2-0.096X_1X_2 \quad (4.5)$$

$$\Delta n_D = -1.55002+0.01008X_1-0.00002X_1^2-0.07510X_2+0.06440X_2^2+0.00002X_1X_2 \quad (4.6)$$

The positive indicator reflects the synergistic influence, while the negative indicator denotes the antagonistic impact of the system parameters on the corresponding responses.

Table 4.7. ANOVA for Excess molar volume, Viscosity deviation, Ultrasonic velocity deviation and Refractive index deviation of acetophenone and cis-3-hexenyl isobutyrate binary mixture

	Source	Sum of squares	Degree of freedom	Mean square	F value	p-value Prob > F
Excess molar volume	X_1-T	0.000132	1	0.000132	9.90917	0.034584
	X_1^2	0.000074	1	0.000074	5.53936	0.078209
	X_2-X	0.000026	1	0.000026	1.93373	0.236720
	X_2^2	0.000707	1	0.000707	52.98433	0.001893
	X1X2	0.000025	1	0.000025	0.02476	0.882581
	R-squared = 0.95017					

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	Adj R-squared = 0.88788					
Viscosity deviation	X_1-T	0.000232	1	0.000232	15.2334	0.017497
	X_1^2	0.000001	1	0.000001	0.0417	0.848226
	X_2-X	0.000116	1	0.000116	7.6287	0.050744
	X_2^2	0.003441	1	0.003441	226.0070	0.000114
	X1X2	0.000046	1	0.000046	0.0262	0.879356
	R-squared = 0.98409					
	Adj R-squared = 0.96421					
Ultrasonic velocity deviation	X_1-T	26.7878	1	26.7878	115.912	0.000422
	X_1^2	1.4866	1	1.4866	6.432	0.064238
	X_2-X	21.5822	1	21.5822	93.387	0.000641
	X_2^2	852.6031	1	852.6031	3689.253	0.000000
	X1X2	0.5675	1	0.5675	2.456	0.192162
	R-squared = 0.99897					
	Adj R-squared = 0.99768					
Refractive index deviation	X_1-T	0.000013	1	0.000013	10.4716	0.031794
	X_1^2	0.000006	1	0.000006	4.9418	0.090308
	X_2-X	0.000007	1	0.000007	5.5741	0.077583
	X_2^2	0.000206	1	0.000206	163.4216	0.000216
	X1X2	0.000001	1	0.000001	0.0288	0.873508
	R-squared = 0.9776					
	Adj R-squared = 0.94961					

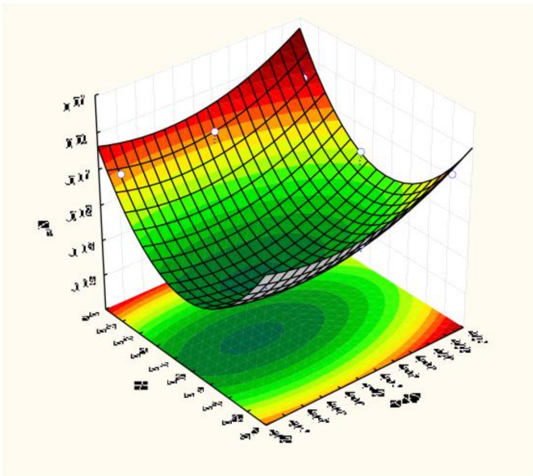

Figure 4.8. Significant combined effect on excess molar volume of acetophenone and cis-3- hexenyl isobutyrate binary mixture ($V^E = cm^3mol^{-1}$)

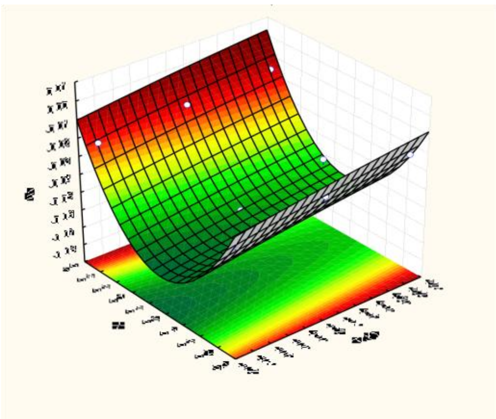

Figure 4.9. Significant combined effect on viscosity deviations of acetophenone and cis3- hexenyl isobutyrate binary mixture (Δη = mPa·s)

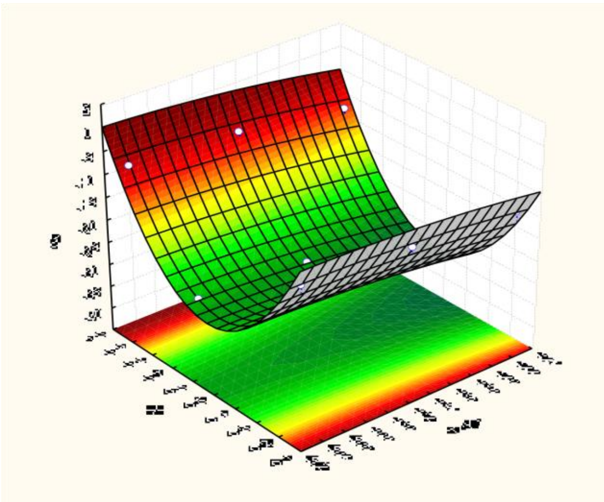

Figure 4.10. Significant combined effect on ultrasonic velocity deviations of acetophenone and cis-3-hexenyl isobutyrate binary mixture (Δu = ms^{-1})

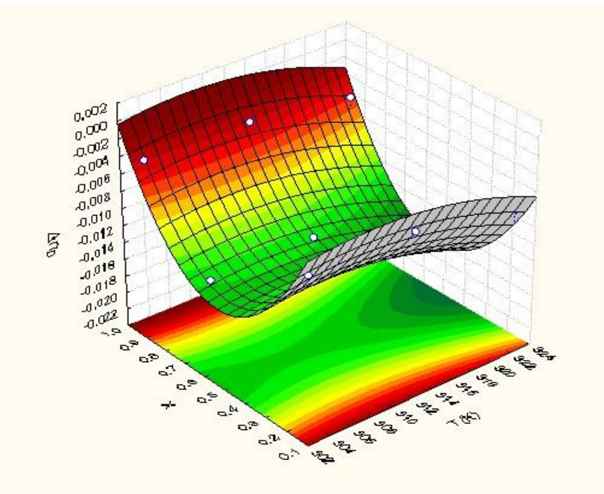

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Figure 4.11. Significant combined effect on refractive index deviations of acetophenone and cis-3-hexenyl isobutyrate binary mixture

The graphical representations of the response surfaces for excess molar volume, viscosity deviation, refractive index deviation, and ultrasonic velocity deviation are illustrated in Figures 4.9, 4.10, 4.11, and 4.12, respectively. Figure 4.55 illustrates that an increase in mole fraction leads to fluctuations in ultrasonic velocity deviation, while a rise in temperature corresponds to a reduction in ultrasonic velocity deviation. In a comparable manner, the variations in viscosity and the discrepancies in refractive index exhibited a trend akin to that observed earlier.

5. DISCUSSION

The systematically negative excess thermophysical properties (VE: -0.033 to 0 $cm^3 \cdot mol^{-1}$, Δη: -0.072 to 0 mPa·s, ΔnD: -0.034 to 0, Δu: -34 to 0 $m \cdot s^{-1}$) across the entire composition range and temperatures (303.15-323.15 K) provide compelling evidence of dominant hetero-molecular attractive forces between acetophenone's electron-rich phenyl ring and carbonyl group with cis-3-hexenyl isobutyrate's polar ester functionality [Rathnam et al., 2012][Nikam & Mehdi, 2002]. These negative deviations signify significant volume contraction and enhanced cohesion, primarily driven by dipole-dipole interactions, π-electron polarization, and efficient interstitial accommodation of the compact ketone within the flexible unsaturated ester chain. The observed temperature dependence—less negative deviations at elevated temperatures—demonstrates thermal disruption of these molecular complexes, consistent with increased kinetic energy weakening dipole associations [Gowrisankar et al., 2015][Gomes, 2024]. Concurrently, negative acoustical impedance deviations (ΔZ: -63 to 0 $kg \cdot m^{-2} \cdot s^{-1}$) coupled with positive intermolecular free length (ΔLf: 0 to 0.10 × 10^{11} m) and isentropic compressibility changes (Δβs: 0 to 0.13 TPa^{-1}) validate Jacobson (1952) theory, confirming increased molecular cohesion alongside local free volume expansion due to structural reorganization [Jacobson, 1952][Mehra & Saini, 2000].

Redlich-Kister polynomial expansions demonstrate exceptional fitting precision (SVE = 0.0008 $cm^3 \cdot mol^{-1}$ at 303.15 K, SΔZ ≤ 1.48 $kg \cdot m^{-2} \cdot s^{-1}$), successfully capturing the asymmetric composition dependence characteristic of polar-nonpolar systems through higher-order coefficients (A3-A5) [Redlich & Kister, 1948]. The Jouyban-Acree model's predictive accuracy for primary properties (Sρ = 0.0012 $g \cdot cm^{-3}$, Sη = 0.0022-0.0032 mPa·s) establishes its reliability for fragrance industry applications where exhaustive experimentation proves impractical [Jouyban & Acree, 2018][Patel, 2023]. Statistical ANOVA validation reveals robust model performance ($R^2 > 0.95$ overall, Fmax = 3689.253 for Δu, $p < 0.05$), with quadratic composition terms (X^2) exerting dominant influence across all responses, underscoring pronounced non-linear molecular interactions [Box & Draper, 1987][Montgomery, 2017]. Response surface equations (4.3-4.6) exhibit high fidelity, enabling interpolation across unmeasured conditions critical for process optimization [Kumar, 2025].

These observations align with Prigogine-Flory-Patterson theory predictions for ketone-ester systems, where equation-of-state contributions favor negative VE while free volume terms partially counteract this effect [Khan et al., 2023]. The positive degree of intermolecular attraction (α < 0) further quantifies enhanced internal pressure in mixed states [Eyring & Kincaid, 1940]. For fragrance formulation, negative excess properties indicate blending volume efficiencies beneficial for cost optimization, while ultrasonic insights support non-invasive quality control through velocity-composition-temperature correlations [Deepthi et al., 2022]. Thermoacoustic parameters enable precise modeling of acoustic mixing processes, crucial for homogenizing viscous flavor concentrates. The empirical polynomials provide immediate design utility, bridging experimental gaps in industrially-relevant temperature-composition space for sustainable process engineering [Sravani et al., 2021].

6. CONCLUSION

This comprehensive study systematically characterizes the thermophysical and thermoacoustic properties of

Acetophenone (1) + cis-3-hexenyl isobutyrate (2) binary mixtures across the full composition range at 303.15, 313.15, and 323.15 K. Experimental measurements reveal consistently negative excess molar volumes (VE: -0.033 to 0 $cm^3 \cdot mol^{-1}$), viscosity deviations (Δη: -0.072 to 0 mPa·s), refractive index deviations (ΔnD: -0.034 to 0), and ultrasonic velocity deviations (Δu: -34 to 0 $m \cdot s^{-1}$), confirming strong intermolecular attractions dominated by dipole-dipole and π-electron interactions between the aromatic ketone and aliphatic ester functionalities. Derived thermoacoustic parameters exhibit negative acoustical impedance deviations (ΔZ: -63 to 0 $kg \cdot m^{-2} \cdot s^{-1}$), positive intermolecular free length changes (ΔLf: 0 to 0.10 × 10^{11} m), and positive isentropic compressibility deviations (Δβs: 0 to 0.13 TPa^{-1}), indicating enhanced molecular packing efficiency and cohesive forces with increasing acetophenone content. Redlich-Kister polynomials provide excellent fits ($S \leq 1.48$ $kg \cdot m^{-2} \cdot s^{-1}$ for ΔZ), while Jouyban-Acree models accurately predict primary properties (Sρ ≈ 0.0012 $g \cdot cm^{-3}$). ANOVA validates empirical response surface models ($R^2 > 0.95$, Fmax = 3689.253, $p < 0.05$), confirming significant temperature-composition interactions for industrial process design in fragrance formulations. These findings elucidate molecular association patterns essential for flavoring agent optimization and thermodynamic modeling.

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