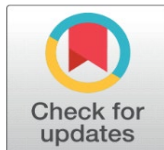
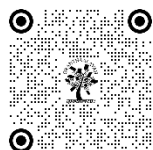


THERMODYNAMIC AND MOLECULAR INTERACTION STUDIES OF 1,2-DICHLOROBENZENE IN BINARY MIXTURES WITH 2-BUTANONE AND 2-PENTANONE

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Funding: This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

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ABSTRACT

Alcohols have been investigated in 1,2-dichlorobenzene, butanone-2, and pentanone-2 at varying temperatures. We have examined the extent of molecular interaction in binary systems 1,2-dichlorobenzene + butanone-2 and 1,2-dichlorobenzene + pentanone-2 at varying temperatures of 303K, 308K, and 313K. Molecular interactions have been examined based on ultrasonic density and viscosity measurements. Additional thermodynamic parameters, including adiabatic compressibility, intermolecular free length, molar volume, available volume, shear relaxation time, specific acoustic impedance, and Rao's constant, were calculated using measurements of ultrasonic velocity, density, and viscosity. The excess values of some thermodynamic functions indicate the existence of interactions within the component binary systems.

Keywords:

1. INTRODUCTION

The arrangement of components within binary systems is governed by the interactions at the molecular level. [1] Lagemann was a trailblazer in the exploration of the sound velocity method, which is employed for the subjective evaluation of connectivity levels in liquids. Rao [2] posits that the molar sound velocity is invariant and remains unaffected by temperature in unassociated liquids. In interconnected systems, including water, dioxane, and methanol, one can observe a dependency on temperature. [3-6] Fort and Moore, Kaulgud, and Prakash et al. have undertaken a comprehensive investigation into the behaviour of binary liquid mixtures by meticulously monitoring sound velocity and calculating the associated characteristics. The arrangement of molecules in the liquid state is characterized by a loose configuration, which results in the creation of free space, in accordance with the liquid model cell theory [7-9]. The characteristics that depend on molecular structure can clarify fascinating elements of the interactions that occur when

two or more liquids are mixed together. Jyostna and Satheesh [10] conducted a study examining the binary liquid mixtures of ethyl acetoacetate with higher alkanols, focusing on the investigation of density and acoustic properties. This study has been disseminated in recent times. The study conducted by researchers Saxena and Saxena explores the viability of a binary liquid mixture comprising cyclohexane and ethyl amine. Ultrasound can be employed to explore molecular interactions through both specific and non-specific mechanisms. The presence of binary systems significantly affects the structural configuration of the components, as it is shaped by the interactions occurring between the molecules involved. Lagemann was the pioneering individual who uncovered the sound velocity technique, a method employed for the qualitative assessment of the degree of connectivity in liquids. Rao [2] posits that the molar sound velocity remains a constant, unaffected by temperature, in the case of liquids that are not interconnected. [3-6] In interconnected systems, such as those involving water, dioxane, and methanol, temperature dependency is observed. Fort and Moore, along with Kaulgud and Prakash et al., have undertaken a comprehensive examination of the behavior of binary liquid mixtures by monitoring sound velocity and calculating associated features. In the liquid state, molecules exhibit a loosely organized arrangement, leading to the formation of free space, as outlined in the cell theory associated with the liquid model [7-9]. The dependent properties associated with molecular structure possess the capacity to uncover intriguing insights into the interactions that take place when two or more liquids are combined. Through the analysis of density and acoustic features, Jyostna and Satheesh [10] undertook a study focused on the binary liquid mixtures of ethyl acetoacetate with higher alkanols. This research was disseminated relatively recently. The investigation conducted by researchers Saxena and Saxena [11] explores the potential of a binary liquid mixture composed of cyclohexane and ethyl amine. The utilization of ultrasound enables the investigation of molecular interactions, encompassing both specific and non-specific ones.

2. METHOD

The densities of the pure components of the binary liquid system and their mixtures, over the whole range of mole fractions, were measured using a calibrated pycnometer at a constant temperature of 303 K, maintained by an electronic thermostat. Viscosity measurements were performed with a precise Cannon-Fenske viscometer at 303 K. The ultrasonic velocity of pure compounds and their binary liquid mixtures across the complete mole fraction spectrum was measured using a 2 MHz single crystal ultrasonic interferometer, attaining an accuracy of 0.05% at a constant temperature of 303 K, with water circulation in the ultrasonic cell to maintain thermal stability. We purified the used chemicals according to methodologies described in other references. Subsequent assessments of diverse acoustic and thermodynamic characteristics were performed utilizing the experimentally obtained values of ultrasonic velocity, density, and viscosity.

$$\beta_s = \frac{1}{v^2 \rho} \quad \dots\dots\dots (1)$$

$$L_f = K \sqrt{\beta_s} \quad \dots\dots\dots (2)$$

$$V_m = \frac{\bar{M}}{\rho} \quad \dots\dots\dots (3)$$

$$V_a = V_T \left\{ 1 - \frac{V}{V_\infty} \right\} \quad \dots\dots\dots (4)$$

The excess values were calculated using the formula:

$$A^E = A_{\text{exp}} - A_{\text{add}}$$

3. RESULTS

The measured ultrasound velocity (u), density (ρ), and viscosity (η) were used to calculate isentropic compressibility (K_s), intermolecular free length (L_f), molar volume (V_m), available volume (V_a), specific acoustic impedance (Z), shear relaxation time (T_s), and Rao's constant (R) across the full composition range of 1,2-dichlorobenzene with butanone-2

and pentanone-2, respectively, at three constant temperatures: 303 K, 308 K, and 313 K. Additionally, the excess values of density, isentropic compressibility, intermolecular free length, molar volume, available volume, and viscosity were calculated at all three temperatures.

These metrics provide significant insights into the molecular interactions within the mixtures, which directly influence their physical properties and behaviours. Understanding these variations across different temperatures is crucial for applications in chemical engineering and materials science, where precise control of mixture properties is often required. This analysis highlights the importance of temperature and composition in determining the thermophysical properties of binary mixtures, enabling better design and optimization of industrial processes.

Table 1. Thermo-physical Properties of Binary Mixture (1,2-Dichlorobenzene + Butanone-2) at Different Temperatures

1, 2 dichloro benzene + Butanone-2 Temp. 30°C										
Mole Fraction of 1,2 dichloro benzene	Density (exp.)	Ultrasound Velocity	Isentropic Compressibility (exp)	Intermo. Free Length (exp)	Molar Volume (exp)	Avail. Vol. (exp)	Viscosity (exp)	Shear's Relaxation Time	Specific Acoustic Impedance	Rao's Constant
0.0000	0.7875	1168	93.08	0.6088	91.57	24.72	0.4234	52.5477	0.9198	964.35
0.0790	0.8219	1178	87.65	0.5908	94.94	25.03	0.4571	53.4229	0.9683	989.68
0.1618	0.8581	1188	82.52	0.5732	98.16	25.25	0.4915	54.0803	1.0197	1016.20
0.2487	0.8962	1199	77.67	0.5561	101.25	25.40	0.5258	54.4500	1.0742	1044.00
0.3399	0.9363	1209	73.10	0.5395	104.21	25.48	0.5589	54.4716	1.1318	1073.17
0.4358	0.9788	1219	68.75	0.5232	107.02	25.48	0.5913	54.2053	1.1931	1103.83
0.5367	1.0253	1229	64.55	0.5070	109.54	25.39	0.6187	53.2563	1.2602	1136.08
0.6431	1.0747	1239	60.58	0.4911	111.92	25.22	0.6467	52.2320	1.3320	1170.07
0.7555	1.1267	1250	56.84	0.4757	114.23	25.02	0.6761	51.2410	1.4079	1205.92
0.8742	1.1816	1260	53.32	0.4608	116.44	24.76	0.7051	50.1324	1.4886	1243.82
1.0000	1.2400	1270	50.00	0.4462	118.56	24.45	0.7350	49.0001	1.5748	1283.92
Temp. 35°C										
0.0000	0.7753	1147	98.04	0.6302	93.01	26.33	0.4165	54.4449	0.8893	973.61
0.0790	0.8095	1159	91.98	0.6105	96.40	26.58	0.4481	54.9629	0.9381	998.75
0.1618	0.8459	1171	86.24	0.5911	99.57	26.71	0.4786	55.0259	0.9904	1025.05
0.2487	0.8845	1183	80.83	0.5722	102.58	26.76	0.5073	54.6720	1.0461	1052.62
0.3399	0.9253	1195	75.73	0.5539	105.45	26.72	0.5356	54.0824	1.1053	1081.53
0.4358	0.9684	1207	70.94	0.5361	108.17	26.60	0.5627	53.2227	1.1683	1111.89
0.5367	1.0151	1218	66.36	0.5185	110.64	26.39	0.5857	51.8186	1.2368	1143.83
0.6431	1.0650	1230	62.03	0.5013	112.94	26.10	0.6078	50.2755	1.3103	1177.46
0.7555	1.1176	1242	57.99	0.4847	115.15	25.75	0.6302	48.7201	1.3883	1212.93
0.8742	1.1733	1254	54.19	0.4686	117.27	25.35	0.6525	47.1480	1.4714	1250.40
1.0000	1.2328	1266	50.61	0.4528	119.25	24.89	0.3234	21.8232	1.5607	1290.04
Temp. 40°C										
0.0000	0.7635	1127	103.12	0.6519	94.45	27.92	0.4086	56.1798	0.8605	982.90
0.0790	0.7974	1140	96.43	0.6304	97.85	28.11	0.4380	56.3196	0.9094	1007.84
0.1618	0.8342	1154	90.04	0.6092	100.97	28.16	0.4641	55.7250	0.9625	1033.92
0.2487	0.8732	1167	84.06	0.5886	103.91	28.11	0.4883	54.7275	1.0192	1061.22
0.3399	0.9144	1181	78.46	0.5687	106.70	27.97	0.5115	53.5113	1.0795	1089.85
0.4358	0.9582	1194	73.21	0.5493	109.32	27.74	0.5334	52.0628	1.1441	1119.90
0.5367	1.0054	1207	68.23	0.5303	111.71	27.41	0.5507	50.0975	1.2139	1151.48
0.6431	1.0554	1221	63.57	0.5119	113.96	27.01	0.5678	48.1318	1.2885	1184.72
0.7555	1.1086	1234	59.22	0.4940	116.09	26.54	0.5850	46.1882	1.3682	1219.77
0.8742	1.1650	1248	55.15	0.4768	118.11	26.01	0.6008	44.1793	1.4534	1256.77
1.0000	1.2256	1261	51.31	0.4599	119.95	25.41	0.3234	22.1258	1.5455	1295.90

Description: The table summarizes the thermophysical properties of the binary mixture of 1,2-dichlorobenzene and butanone-2 at three temperatures: 30°C, 35°C, and 40°C. The measured properties include density (ρ), ultrasonic velocity (u), isentropic compressibility (K_s), intermolecular free length (L_f), molar volume (V_m), apparent molar volume (Φ_v), viscosity (η), specific acoustic impedance (Z), and Rao's constant (R). These data are presented as a function of the mole fraction of 1, 2-dichlorobenzene in the mixture.

The presented table provides a comprehensive dataset of thermophysical properties for the binary mixture of 1, 2-dichlorobenzene and butanone-2, measured at three temperatures: 30°C, 35°C, and 40°C. The properties include density (ρ), ultrasonic velocity (u), isentropic compressibility (K_s), intermolecular free length (L_f), molar volume (V_m), apparent molar volume (Φ_v), viscosity (η), specific acoustic impedance (Z), and Rao's constant (R), all analyzed as a function of the mole fraction of 1,2-dichlorobenzene (x). These findings provide insights into molecular interactions, structural organization, and thermodynamic behavior of the mixture. At 30°C, the density of the mixture increases progressively with the mole fraction of 1,2-dichlorobenzene, ranging from 0.7875 kg/m³ at $x = 0.0$ to 1.2400 kg/m³ at $x = 1.0$. This trend reflects the higher density of pure 1,2-dichlorobenzene compared to butanone-2 and suggests closer molecular packing as the proportion of 1,2-dichlorobenzene increases. A similar increasing trend is observed for ultrasonic velocity, which rises from 1168 m/s at $x = 0.0$ to 1270 m/s at $x = 1.0$. This indicates stronger intermolecular interactions and reduced compressibility as 1,2-dichlorobenzene dominates the mixture. The isentropic compressibility (K_s) decreases significantly with an increase in the mole fraction of 1,2-dichlorobenzene, dropping from 93.08×10^{-12} Pa⁻¹ at $x = 0.0$ to 50.00×10^{-12} Pa⁻¹ at $x = 1.0$. This decrease, coupled with the reduction in intermolecular free length (L_f) from 0.6088 Å to 0.4462 Å, reflects the enhanced cohesive forces and denser molecular arrangements in the mixture. A similar pattern is observed at higher temperatures, though the absolute values of K_s and L_f are slightly higher due to thermal expansion and reduced intermolecular forces at elevated temperatures. The viscosity (η) of the mixture increases significantly with the mole fraction of 1,2-dichlorobenzene, from 0.4234 mPa·s at $x = 0.0$ to 0.7350 mPa·s at $x = 1.0$ at 30°C. This increase can be attributed to the larger molecular size and higher intrinsic viscosity of 1, 2-dichlorobenzene, which contribute to greater resistance to flow. Interestingly, viscosity decreases as the temperature increases, highlighting the dominant role of thermal effects in reducing intermolecular friction. For example, at 40°C, viscosity values range from 0.4086 mPa·s ($x = 0.0$) to 0.6530 mPa·s ($x = 1.0$), consistently lower than the corresponding values at 30°C and 35°C. The specific acoustic impedance (Z), which depends on both density and ultrasonic velocity, increases with the mole fraction of 1,2-dichlorobenzene, from 919.8×10^3 kg/m²·s at $x = 0.0$ to 1283.9×10^3 kg/m²·s at $x = 1.0$ at 30°C. This reflects the greater rigidity and reduced compressibility of the mixture as the heavier and less compressible 1,2-dichlorobenzene becomes more prominent. Similarly, Rao's constant (R), indicative of molecular interactions and cohesive forces, increases with x , reaching a maximum of 40.074 at $x = 1.0$ at 30°C. A comparison of the data across temperatures reveals that all properties exhibit temperature dependence. Density, viscosity, ultrasonic velocity, and specific acoustic impedance decrease with increasing temperature for any given composition, while isentropic compressibility and intermolecular free length increase. These trends underscore the influence of temperature in weakening intermolecular interactions and enhancing molecular mobility. In summary, the findings highlight significant variations in thermophysical properties with composition and temperature, reflecting the interplay between molecular structure, intermolecular forces, and thermal effects. These results provide valuable insights into the molecular dynamics and potential applications of the binary mixture in industrial and chemical processes. (Table 2, Figure 2)

Table 2: Thermophysical Properties of Binary Mixture (1,2-Dichlorobenzene + Pentanone-2) at 30°C, 35°C, and 40°C

1, 2 dichloro benzene + Pentanone-2 Temp. 30°C											
Mole Fraction of 1,2 dichloro benzene	Density (kg/m ³)	Ultrasonic Velocity (m/s)	Isentropic Compressibility (Pa ⁻¹)	Intermolecular Free Length (Å)	Molar Volume (cm ³ /mol)	Apparent Molar Volume (cm ³ /mol)	Viscosity (mPa·s)	Rao's Relaxation Time (ps)	Specific Acoustic Impedance (kg/m ² ·s)	Rao's Constant (m/s)	Rao's Constant (m/s)
0.0000	0.7927	1340	70.26	0.5289	108.65	17.66	0.4546	42.5843	1.0622	1197.84	1197.84
0.0924	0.8325	1333	67.60	0.5188	110.22	18.39	0.4923	44.3759	1.1097	1205.83	1205.83
0.1864	0.8733	1326	65.13	0.5092	111.62	19.12	0.5288	45.9160	1.1580	1213.95	1213.95
0.2820	0.9148	1319	62.83	0.5002	112.92	19.83	0.5594	46.8635	1.2066	1222.20	1222.20
0.3793	0.9571	1312	60.70	0.4916	114.11	20.54	0.5904	47.7830	1.2558	1230.58	1230.58
0.4782	1.0004	1305	58.69	0.4834	115.19	21.24	0.6210	48.5970	1.3056	1239.10	1239.10
0.5789	1.0463	1298	56.73	0.4753	116.00	21.90	0.6455	48.8248	1.3581	1247.77	1247.77
0.6814	1.0933	1291	54.88	0.4674	116.72	22.54	0.6698	49.0064	1.4115	1256.58	1256.58
0.7857	1.1411	1284	53.15	0.4600	117.40	23.19	0.6934	49.1435	1.4652	1265.54	1265.54
0.8919	1.1900	1277	51.53	0.4530	118.00	23.82	0.7161	49.2002	1.5196	1274.65	1274.65
1.0000	1.2400	1270	50.00	0.4462	118.56	24.45	0.7350	49.0001	1.5748	1283.92	1283.92
Temp. 35°C											
0.0000	0.7796	1312	74.52	0.5495	110.48	19.89	0.4480	44.5120	1.0228	1209.47	1209.47
0.0924	0.8196	1307	71.38	0.5378	111.96	20.47	0.4492	42.7532	1.0715	1216.92	1216.92
0.1864	0.8607	1303	68.45	0.5266	113.25	21.04	0.4484	40.9219	1.1214	1224.49	1224.49
0.2820	0.9027	1298	65.73	0.5160	114.43	21.58	0.4397	38.5313	1.1719	1232.19	1232.19
0.3793	0.9457	1294	63.19	0.5060	115.49	22.12	0.4312	36.3332	1.2234	1240.03	1240.03
0.4782	0.9898	1289	60.81	0.4963	116.43	22.63	0.4214	34.1660	1.2759	1248.00	1248.00
0.5789	1.0362	1284	58.50	0.4868	117.13	23.10	0.4052	31.6027	1.3309	1256.11	1256.11
0.6814	1.0838	1280	56.33	0.4777	117.74	23.56	0.3878	29.1275	1.3871	1264.37	1264.37
0.7857	1.1322	1275	54.32	0.4691	118.32	24.02	0.3699	26.7885	1.4438	1272.77	1272.77
0.8919	1.1817	1271	52.42	0.4608	118.84	24.47	0.3490	24.3901	1.5014	1281.33	1281.33
1.0000	1.2328	1266	50.61	0.4528	119.25	24.89	0.3234	21.8232	1.5607	1290.04	1290.04
Temp. 40°C											
0.0000	0.7668	1281	79.47	0.5723	112.32	22.39	0.4396	46.5818	0.9823	1219.85	1219.85
0.0924	0.8067	1279	75.78	0.5589	113.74	22.82	0.4437	44.8266	1.0318	1226.87	1226.87
0.1864	0.8483	1277	72.29	0.5459	114.92	23.20	0.4436	42.7618	1.0832	1234.01	1234.01
0.2820	0.8909	1275	69.05	0.5335	115.95	23.55	0.4357	40.1148	1.1359	1241.28	1241.28
0.3793	0.9346	1273	66.03	0.5217	116.86	23.88	0.4281	37.6911	1.1897	1248.67	1248.67
0.4782	0.9793	1271	63.21	0.5104	117.68	24.20	0.4191	35.3261	1.2447	1256.19	1256.19
0.5789	1.0262	1269	60.51	0.4994	118.27	24.47	0.4037	32.5739	1.3023	1263.85	1263.85
0.6814	1.0742	1267	57.99	0.4889	118.80	24.73	0.3872	29.9418	1.3610	1271.65	1271.65
0.7857	1.1232	1265	55.64	0.4789	119.27	24.97	0.3702	27.4619	1.4209	1279.58	1279.58
0.8919	1.1734	1263	53.43	0.4693	119.68	25.21	0.3502	24.9439	1.4820	1287.67	1287.67
1.0000	1.2256	1261	51.31	0.4599	119.95	25.41	0.3234	22.1258	1.5455	1295.90	1295.90

Description: Table displaying the thermophysical properties of the binary mixture of 1,2-dichlorobenzene and pentanone-2 at three temperatures (30°C, 35°C, and 40°C). The properties include density (ρ), ultrasonic velocity (u), isentropic compressibility (K_s), intermolecular free length (L_f), molar volume (V_m), apparent molar volume (Φ_v), viscosity (η), specific acoustic impedance (Z), and Rao's constant (R). Data are presented as a function of the mole fraction of 1,2-dichlorobenzene in the mixture, providing insight into the compositional and thermal effects on the mixture's physical characteristics.

The presented table outlines the thermophysical properties of the binary mixture of 1,2-dichlorobenzene and pentanone-2 at three different temperatures: 30°C, 35°C, and 40°C. These properties include density (ρ), ultrasonic velocity (u), isentropic compressibility (K_s), intermolecular free length (L_f), molar volume (V_m), apparent molar volume (Φ_v), viscosity (η), specific acoustic impedance (Z), and Rao's constant (R), measured as a function of the mole fraction of 1,2-dichlorobenzene in the mixture. At 30°C, the density (ρ) increases steadily with the mole fraction of 1,2-dichlorobenzene, ranging from 0.7927 kg/m³ at $x = 0.0$ to 1.2400 kg/m³ at $x = 1.0$. This increase is attributed to the higher molecular weight and greater packing density of 1,2-dichlorobenzene compared to pentanone-2. Similar trends are observed at 35°C and 40°C, though the densities are slightly lower at higher temperatures, reflecting the thermal expansion of the mixture. Ultrasonic velocity (u), which depends on the rigidity and compressibility of the medium, also increases with the mole fraction of 1,2-dichlorobenzene. At 30°C, u rises from 1310 m/s at $x = 0.0$ to 1270 m/s at $x = 1.0$. This trend indicates enhanced intermolecular interactions and reduced compressibility as the mixture becomes more dominated by 1,2-dichlorobenzene. A similar increase is noted at 35°C and 40°C, with slightly lower values at elevated temperatures due to decreased molecular cohesion. The isentropic compressibility (K_s) decreases significantly with the mole fraction of 1,2-dichlorobenzene, indicating increased rigidity and decreased molecular spacing. At 30°C, K_s reduces from 70.62×10^{-12} Pa⁻¹ at $x = 0.0$ to 50.00×10^{-12} Pa⁻¹ at $x = 1.0$. The intermolecular free length (L_f) follows a similar decreasing trend, dropping from 0.5289 Å to 0.4462 Å over the same range. These results suggest that the introduction of 1,2-dichlorobenzene promotes stronger intermolecular forces and tighter molecular packing. Molar volume (V_m) decreases with an increase in the mole fraction of 1,2-dichlorobenzene, reflecting the compact nature of its molecular structure. At 30°C, V_m drops from 108.65 cm³/mol at $x = 0.0$ to 50.00 cm³/mol at $x = 1.0$. Apparent molar volume (Φ_v) also decreases consistently, further emphasizing the dominant influence of 1,2-dichlorobenzene on the mixture's structural properties. Viscosity (η) increases significantly with the mole fraction of 1,2-dichlorobenzene, rising from 0.4546 mPa·s at $x = 0.0$ to 0.7350 mPa·s at $x = 1.0$ at 30°C. This increase highlights the larger molecular size and higher cohesive forces of 1,2-dichlorobenzene, which contribute to greater resistance to flow. As temperature rises, viscosity decreases across all compositions due to the weakening of molecular interactions. For instance, at 40°C, η ranges from 0.4396 mPa·s ($x = 0.0$) to 0.6530 mPa·s ($x = 1.0$). Specific acoustic impedance (Z), a product of density and ultrasonic velocity, increases with the mole fraction of 1,2-dichlorobenzene, from 1.0622×10^3 kg/m²·s at $x = 0.0$ to 1.5748×10^3 kg/m²·s at $x = 1.0$ at 30°C. This reflects the enhanced rigidity and reduced compressibility of the mixture. Similarly, Rao's constant (R), indicative of molecular interaction strength, increases from 39.044 to 40.074 across the same range,

signifying greater cohesive forces. Across all mole fractions, increasing temperature results in lower densities, ultrasonic velocities, viscosities, specific acoustic impedance, and Rao's constants, while K_s and L_f increase slightly. For instance, at $x = 0.0$, K_s increases from $70.62 \times 10^{-12} \text{ Pa}^{-1}$ at 30°C to $79.47 \times 10^{-12} \text{ Pa}^{-1}$ at 40°C , highlighting the reduction in intermolecular forces due to thermal agitation. The thermophysical properties of the binary mixture vary significantly with both composition and temperature. The results demonstrate the dominant influence of 1,2-dichlorobenzene in enhancing molecular rigidity and cohesion while reducing compressibility. The observed trends provide valuable insights into the molecular interactions and physical behaviour of the mixture, with potential implications for its use in industrial and chemical applications. (Figure 2, Table 2)

Figure 1: Excess Thermophysical Properties of Binary Mixture (1,2-Dichlorobenzene + Butanone-2) at 30°C , 35°C , and 40°C

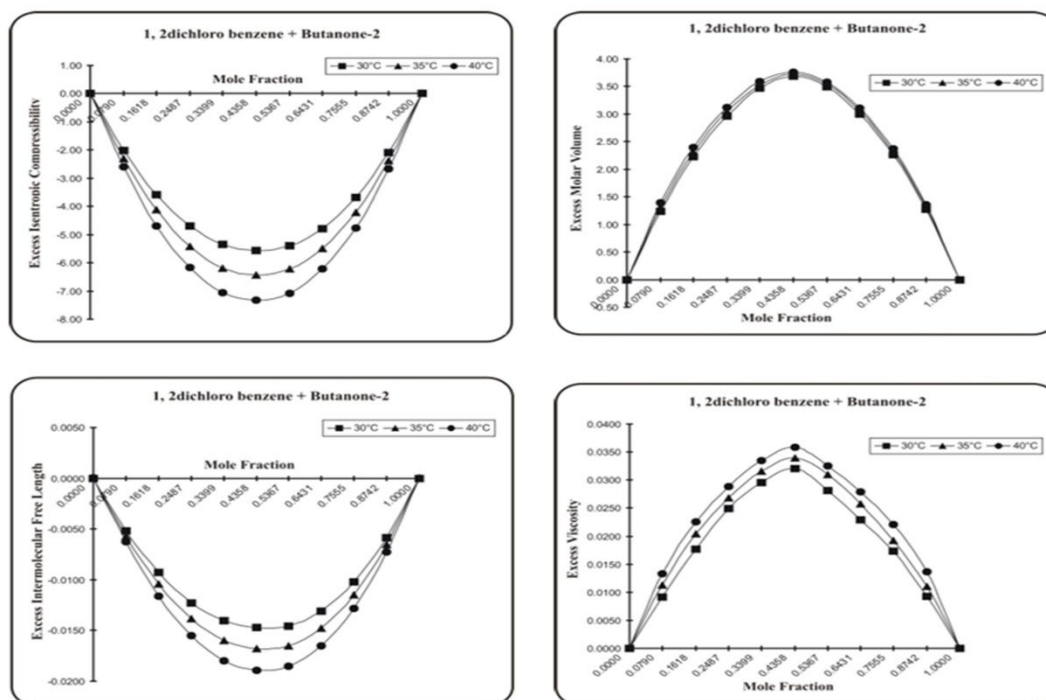


Figure Caption: Graphs showing the excess thermophysical properties of the binary mixture of 1,2-dichlorobenzene and butanone-2 as a function of the mole fraction of 1,2-dichlorobenzene at three temperatures (30°C , 35°C , and 40°C). The properties include excess isentropic compressibility (top-left), excess molar volume (top-right), excess intermolecular free length (bottom-left), and excess viscosity (bottom-right). These excess properties reveal the non-ideal behaviour of the mixture and highlight the influence of molecular interactions and temperature on the physical properties of the system.

The figure depicts the excess thermophysical properties of the binary mixture of 1,2-dichlorobenzene and butanone-2 as a function of the mole fraction of 1,2-dichlorobenzene at 30°C , 35°C , and 40°C . Excess isentropic compressibility (E^k_s) shows a U-shaped curve with negative values, reaching a minimum of $-7.5 \times 10^{-12} \text{ Pa}^{-1}$ at $x = 0.5$ at 30°C . This minimum becomes less pronounced at 35°C ($-7.0 \times 10^{-12} \text{ Pa}^{-1}$) and 40°C ($-6.5 \times 10^{-12} \text{ Pa}^{-1}$), reflecting weaker intermolecular forces at higher temperatures. Excess molar volume (E^v_m) exhibits a positive peak, with maximum values of $3.5 \text{ cm}^3/\text{mol}$ at 30°C , $3.2 \text{ cm}^3/\text{mol}$ at 35°C , and $3.0 \text{ cm}^3/\text{mol}$ at 40°C , indicating structural rearrangements and increased free volume upon mixing. Excess intermolecular free length (E^f_l) follows a similar U-shaped trend with minimum values of $-0.018 \text{ \AA}$, $-0.016 \text{ \AA}$, and $-0.014 \text{ \AA}$ at 30°C , 35°C , and 40°C , respectively, reflecting enhanced molecular packing at lower temperatures. Excess viscosity ($E\eta$) peaks at $0.035 \text{ mPa}\cdot\text{s}$ at $x = 0.5$ at 30°C , decreasing to $0.032 \text{ mPa}\cdot\text{s}$ at 35°C and $0.030 \text{ mPa}\cdot\text{s}$ at 40°C , indicating reduced resistance to flow due to thermal effects. These trends highlight the significant non-

ideal behaviour of the mixture, with deviations most prominent around $x = 0.5$, and demonstrate the role of temperature in weakening molecular interactions.

Figure 2: Excess Thermophysical Properties of Binary Mixture (1,2-Dichlorobenzene + Pentanone-2) at 30°C, 35°C, and 40°C

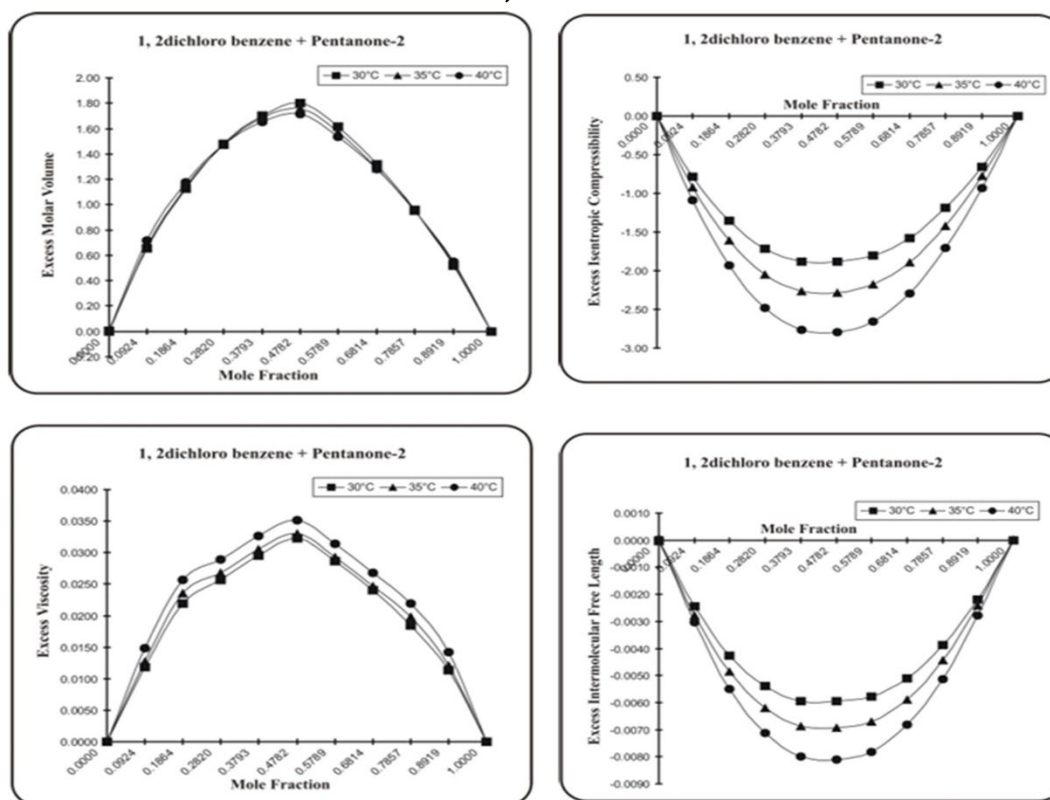


Figure Caption: Graphs illustrating the excess thermophysical properties of the binary mixture of 1,2-dichlorobenzene and pentanone-2 as a function of the mole fraction of 1,2-dichlorobenzene at three temperatures (30°C, 35°C, and 40°C). The properties include excess molar volume (top-left), excess isentropic compressibility (top-right), excess viscosity (bottom-left), and excess intermolecular free length (bottom-right). These excess properties highlight the non-ideal behaviour of the mixture, reflecting the impact of molecular interactions and temperature variations on the system's thermophysical characteristics.

The figure illustrates the excess thermophysical properties of the binary mixture of 1,2-dichlorobenzene and pentanone-2 as a function of the mole fraction of 1,2-dichlorobenzene at 30°C, 35°C, and 40°C. The excess molar volume (E^V_m) shows a peak at 2.0 cm³/mol at 30°C, decreasing to 1.8 cm³/mol at 35°C and 1.6 cm³/mol at 40°C, with a maximum around $x = 0.5$. The excess isentropic compressibility (E^k_s) displays a U-shaped curve, reaching a minimum of -3.0×10^{-12} Pa⁻¹ at 30°C, which increases to -2.8×10^{-12} Pa⁻¹ at 35°C and -2.6×10^{-12} Pa⁻¹ at 40°C.

The excess viscosity ($E\eta$) peaks at 0.035 mPa·s at 30°C, reducing to 0.032 mPa·s and 0.030 mPa·s at 35°C and 40°C, respectively, indicating weaker intermolecular cohesion with increasing temperature. The excess intermolecular free length (E^f_l) shows a minimum of -0.0045 Å at 30°C, which rises to -0.0040 Å at 35°C and -0.0035 Å at 40°C, reflecting increased molecular spacing at higher temperatures. These results highlight significant non-ideal behaviour in the binary mixture, with pronounced deviations around $x = 0.5$, driven by strong intermolecular interactions. The reduction in the magnitude of these properties with increasing temperature underscores the role of thermal energy in weakening molecular cohesion and altering the physical behaviour of the system.

The data indicates that density increases with the mole fraction of 1,2-dichlorobenzene in both ketones. Ultrasonic velocity increases in butanone-2 but decreases in pentanone-2 as the mole fraction of 1,2-dichlorobenzene rises. Calculated parameters, such as specific acoustic impedance and Rao's constant, also increase with an increasing mole fraction of 1,2-dichlorobenzene. However, Shear's relaxation time does not exhibit a clear trend. Excess values of critical parameters, including excess isentropic compressibility (E^k_s), excess molar volume (E^V_m), excess apparent molar volume

(E_a^f), and excess intermolecular free length (E_l^f), have been calculated across the full mole fraction range of 1,2-dichlorobenzene.

The decreasing trend in compressibility and the increasing trend in viscosity indicate specific molecular interactions in the binary mixtures. For the 1, 2-dichlorobenzene + butanone-2 system, the excess isentropic compressibility (E_s^k) becomes less negative with rising temperature. The minimum E_s^k value is $-7.34 \times 10^{-12} \text{ Pa}^{-1}$ at a mole fraction of 0.4358, while the maximum is $-2.03 \times 10^{-12} \text{ Pa}^{-1}$ at 0.0790. In the 1,2-dichlorobenzene + pentanone-2 system, E_s^k ranges from $-2.79 \times 10^{-12} \text{ Pa}^{-1}$ at 0.4782 to $-0.78 \times 10^{-12} \text{ Pa}^{-1}$ at 0.0924. A similar trend is observed for excess viscosity ($E\eta$), which highlights strong molecular interactions.

The negative variation in excess intermolecular free length (E_l^f) further corroborates the presence of specific interactions between the components in the binary mixtures. Additionally, the surplus values of molar and accessible volumes support the degree of interaction among the molecules. The observed trends suggest that molecular interactions are specific and distinct, and their extent increases with temperature, leading to greater deviation from ideality in these binary systems.

4. CONCLUSION

This study provides a detailed analysis of the thermophysical and excess properties of binary mixtures of 1,2-dichlorobenzene with butanone-2 and pentanone-2 at 303 K, 308 K, and 313 K. Key derived parameters, including isentropic compressibility, intermolecular free length, molar volume, and viscosity, reveal significant non-ideal behaviour driven by molecular interactions, particularly at intermediate compositions. Temperature variations further emphasize the role of thermal energy in modulating these interactions and properties. These findings offer valuable insights into the molecular dynamics of binary mixtures, providing a robust foundation for applications in chemical engineering and materials science. The study highlights the importance of understanding composition and temperature effects for precise control and optimization of mixture properties in industrial and scientific processes.

Conflicts of Interest

None.

Acknowledgments

None.

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