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RESEARCH PAPER

APPLIED PHYSICS

Molecular Interactions in Tetrachloroethylene-Cyclohexanone Binary Mixtures: Acoustical and FTIR Investigations at Different Temperatures

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ABSTRACT

The speed of sound (U), density (ρ), and viscosity (η) of binary liquid mixtures of tetrachloroethylene with cyclohexanone, as well as their pure components, were measured across varying mole fractions at four temperatures: 303.15 K, 308.15 K, 313.15 K, and 318.15 K. These experimentally determined physical properties were subsequently used to calculate thermo-acoustic parameters, including excess molar volume (V^E), excess free length (L_f^E), excess Gibbs free energy (ΔG^E), and excess enthalpy (H^E). The observed trends in these parameters were analysed to understand the nature and strength of intermolecular interactions present within the binary mixtures. Additionally, the experimentally measured speed of sound was compared with values predicted by established theoretical models to evaluate their applicability to the system. The models that showed the closest agreement with the experimental data highlighted the presence of specific molecular interactions, such as hydrogen bonding and dipole–dipole interactions, between the components. Further, Fourier Transform Infrared (FTIR) spectroscopy provided detailed insights into the molecular interactions, confirming the presence of structural and chemical effects influencing

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the thermophysical behaviour of the mixtures. The study offers a comprehensive analysis of molecular interactions in tetrachloroethylene–cyclohexanone mixtures across a range of temperatures.

Keywords: Density, Viscosity, Ultrasonic velocity, Excess molar volume, Excess Gibbs free energy, Intermolecular interactions, Binary liquid mixtures, FT-IR spectroscopy

The volumetric and viscometric survey together with Speed of sound of liquid mixtures is significant parameters play a vital role in realizing the intermolecular interactions obtained in and around the molecules. Significant interactions found enormous usage in various manufacturing technological industries(1-7). Diverse scholarly articles found with density, viscosity, and speed of sound calculations for huge range of binary liquid mixtures containing ketones as one of the components(8-13).

Ketones are characterized by the presence of a polar carbonyl (C=O) group, which enables strong dipole–dipole interactions and allows participation in hydrogen-bond-type associations with suitable proton donors (14). Because of these properties, ketones are widely used as solvents and intermediates in chemical synthesis, pharmaceutical formulations, extraction processes, and fine chemical industries. A clear understanding of intermolecular interactions in ketone-containing systems is essential for predicting thermodynamic behavior, phase equilibria, transport properties, and formulation stability(15).

Recent investigations have increasingly emphasized the significance of excess thermodynamic and acoustical parameters in understanding molecular interactions in binary and multicomponent liquid mixtures. Parameters such as excess molar volume, excess compressibility, excess free length, and deviation in ultrasonic velocity are widely used to interpret the strength and nature of intermolecular forces. Theoretical interpretations of such excess functions are strongly supported by classical solution theories, as discussed by Arieh(16). Negative excess values generally indicate strong specific interactions such as hydrogen bonding and dipole–dipole attraction, whereas positive deviations suggest weak dispersive forces and structural loosening within the liquid matrix.

In recent years, computational chemistry has significantly complemented experimental thermodynamic studies. Molecular dynamics simulations, described in detail by Michael(17). Enable the evaluation of radial distribution functions, coordination numbers, and time-dependent molecular arrangements. Similarly, density functional theory (DFT), originally formulated by Walter Kohn and Lu Jeu Sham(18), provides quantum mechanical insight into electronic structure, interaction energies, and hydrogen-bond strength. These modern theoretical tools bridge the gap between macroscopic excess thermodynamic properties and microscopic structural organization.

The combined application of experimental acoustical measurements and theoretical modeling has become particularly valuable in pharmaceutical research, solvent selection, and separation technologies. As highlighted in standard physical chemistry literature by Donald(19), integrating thermodynamic analysis with molecular-level simulations enhances predictive capability and process optimization. Thus, contemporary research increasingly relies on a synergistic approach combining volumetric, ultrasonic, and computational techniques to obtain a comprehensive understanding of molecular association in liquid systems.

The functional parameters of thermodynamics were sensitively depended on various intermolecular forces and on size and shape of molecules(20). From the determined values of speed of sound, viscosity and density we can calculate the excess thermo-acoustic parameters like excess ultrasonic velocity

(U^E), excess adiabatic compressibility (β^E_{ad}), excess molar volume (V^E), excess free length (L_f^E), excess Gibb's free energy (ΔG^E) and excess enthalpy (H^E). Now this current epilogue shows the speed of sound and viscosity values had been a huge empirical bondage with molecular interactions in the liquid. In this paper the results were discussed for liquid mixtures of tetrachloroethylene with cyclohexanone at temperatures (303.15, 308.15, 313.15 and 318.15) K. FT-IR spectra of binary mixtures were obtained at room temperature for different mixtures with pure liquids. The FT-IR spectroscopy is one of the tools to identify the strength of interactions, type of bonding and existence of hydrogen bond with shape and frequency shift of the band.

EXPERIMENTAL

(a) Materials

Tetrachloroethylene (TCE) and cyclohexanone are used in this study. The chemicals of AR grade were purchased from Merck Co. Inc., Germany, with 99% purity (21).

(b) Measurements

The chemical mixtures were kept in observation in air tight bottles 72 hours for measuring viscosity, velocity and density values. Viscosity was measured by using Ostwald viscometer. The uncertainty in viscosity measurement is up to 0.001mPa-s. For measurement of density was accurately using 10 ml specific gravity bottle. The average uncertainty in the measured density is ±0.001 kg/m^3. The speed of sound is measured with a single crystal variable path interferometer operating at a frequency of 2MHz that had been calibrated. The FT/IR-6000 FT-IR spectrometer is used to get the data of binary mixtures.

(c) Computational Details

The values of experimentally determined density and speed of sound for the binary mixtures of tetrachloroethylene with cyclohexanone at 303.15 K, 308.15 K, 313.15 K, and 318.15 K and for different compositions are used to calculate excess parameters.

In the present study the formulas of excess values were calculated by using the expressions given in literature(22) as follows —

Excess free length $L_f^E = L_f - KT\,(Ks)^{1/2}$ ...1

Excess Gibbs free energy $\Delta G^E = \mathrm{RT}\left[\mathrm{In}\left(\frac{\eta V}{\eta_2 V_2}\right) - \mathrm{x}_1\,\mathrm{In}\left(\frac{\eta_1 V_1}{\eta_2 V_2}\right)\right]$ …2

Excess enthalpy $H^E = \mathrm{H} - (x_1 H_1 + x_2 H_2)$ ...3

Excess adiabatic compressibility $\beta^{\mathrm{E}}_{\mathrm{ad}} = \frac{1}{\rho U^2}$ ...4

Excess volume $$V^E = \frac{x_1 M_1 + x_2 M_2}{\rho} - \left(\frac{x_1 M_1}{\rho_1} + \frac{x_2 M_2}{\rho_2}\right) \quad \ldots 5$$

RESULTS AND DISCUSSION

The experimental and literature values of speed of sound (U), density (ρ) and viscosity (η) in pure liquids (Tetrachloroethylene and Cyclohexanone) under study at temperature.

T = 303.15 K are given in **Table 1**

Liquid	**Ultrasonic Velocity (u) m.s^{-1}**		**Density(ρ) x10^{-3} Kgm^{-3}**		**Viscosity(η) × 10^{-3} Ns.m^2**	
	EXP	**LIT**	**EXP**	**LIT**	**EXP**	**LIT**
Tetrachloroethylene	1028.80	1028.80[23]	1606.06	1606.34[24]	0.797	0.798[25,26]
Cyclohexanone	1388.79	1388.00[27]	937.90	937.60[28]	1.8221	1.7571[29]

Table 2*:* The data of density(ρ), speed of sound(U) and viscosity(η), adiabatic compressibility (***β***$_{ad}$), molar volume (V$_m$) and Intermolecular free length (L$_f$) were presented in the below table

Mole Fraction of TCE	**ρ × 10^{-3} Kgm^{-3}**	**U m.s^{-1}**	**η × 10^{-3} Ns.m^2**	**β$_{ad}$ × 10^{-10} kg^{-1}.m s^2**	**L$_f$ ×10^{12} m**	**V$_m$ × 10^{-5} m^3/mol^{-1}**
Tetrachloroethylene + Cyclohexanone at 303.15 K						
0.0000	937.50	1388.79	1.822	5.5303	4.7824	89.7280
0.1478	1045.70	1329.65	1.682	5.5693	4.8083	92.0128
0.3025	1152.40	1272.54	1.525	5.6398	4.8422	94.4703
0.4645	1257.73	1212.24	1.354	5.7202	4.8862	97.0862
0.6343	1363.30	1148.24	1.175	5.8235	4.9452	99.7448
0.8126	1476.24	1089.35	0.991	5.9142	5.0103	102.7713
1.0000	1606.06	1028.80	0.797	6.0103	5.0915	106.0185
Tetrachloroethylene + Cyclohexanone at 313.15 K						
0.0000	933.50	1370.58	1.660	5.7225	4.9220	90.1704
0.1478	1040.60	1311.24	1.534	5.7762	4.9430	92.4609
0.3025	1146.80	1253.35	1.388	5.851	4.9814	94.9273
0.4645	1251.40	1193.25	1.245	5.9363	5.0252	97.5727
0.6343	1356.40	1131.64	1.089	6.0286	5.0826	100.2480
0.8126	1472.14	1072.28	0.932	6.1387	5.1466	103.2523
1.0000	1597.72	1010.80	0.756	6.2245	5.2165	106.4125
Tetrachloroethylene + Cyclohexanone at 313.15 K						
0.0000	929.10	1353.72	1.512	5.9151	5.0495	90.5392
0.1478	1035.50	1292.35	1.387	5.9815	5.0778	92.9046
0.3025	1140.90	1234.34	1.256	6.0749	5.1165	95.4005
0.4645	1245.03	1173.84	1.127	6.1476	5.1632	98.0528
0.6343	1349.40	1112.75	1.001	6.2384	5.2152	100.7962
0.8126	1459.39	1052.69	0.874	6.3425	5.2771	103.8102
1.0000	1589.35	993.00	0.732	6.4474	5.3419	106.8842

Tetrachloroethylene + Cyclohexanone at 318.15 K						
0.0000	924.50	1334.19	1.371	6.1224	5.1875	90.9812
0.1478	1030.30	1272.35	1.252	6.2042	5.2245	93.3429
0.3025	1135.10	1212.65	1.147	6.2950	5.2671	95.8414
0.4645	1238.64	1154.67	1.042	6.3706	5.3041	98.5083
0.6343	1342.30	1094.39	0.930	6.4670	5.3561	101.2414
0.8126	1454.38	1035.38	0.815	6.5796	5.4126	104.2281
1.0000	1580.90	978.26	0.711	6.6864	5.4702	107.3532

Table 3: Values of excess ultrasonic velocity (U^E), excess adiabatic compressibility (β_{ad}^E), excess enthalpy (H^E), excess intermolecular free length (L^{fE}), excess molar volume (), excess Gibb's free energy (ΔG^E) for the binary liquid mixtures of tetrachloroethylene with cyclohexanone at 303.15 to 318.15K

Mole Fraction of TCE	**U^E $m.s^{-1}$**	**$\beta_{ad}^E \times 10^{-10}$ $N^{-1}.m^2$**	**H^E $KJmol^{-1}$**	**$L_f^E \times 10^{12}$ M**	**$V_m^E \times 10^{-5}$ m^3/mol^{-1}**	**$\Delta G^E \times 10^{-20}$ $kJ.mol^{-1}$**
Tetrachloroethylene + Cyclohexanone at 303.15 K						
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1478	-4.7452	-0.2072	0.6402	-0.0920	-0.4030	0.0010
0.3025	-8.5402	-0.3154	0.9915	-0.1432	-0.8350	0.0020
0.4645	-10.5226	-0.3287	0.9454	-0.1585	-1.0745	0.0024
0.6343	-8.8401	-0.2665	0.6760	-0.1425	-0.8525	0.0023
0.8126	-4.7455	-0.1486	0.3356	-0.0924	-0.4456	0.0016
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Tetrachloroethylene + Cyclohexanone at 308.15 K						
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1478	-6.6401	-0.1846	0.7575	-0.0816	-0.4833	0.0009
0.3025	-11.5401	-0.2934	1.2240	-0.1310	-0.9566	0.0018
0.4645	-13.6244	-0.3050	1.2352	-0.1441	-1.1770	0.0022
0.6343	-11.9715	-0.2422	0.9162	-0.1259	-0.9546	0.0021
0.8126	-6.6712	-0.1304	0.4742	-0.0775	-0.5121	0.0014
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Tetrachloroethylene + Cyclohexanone at 313.15 K						
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1478	-8.7401	-0.1612	0.8735	-0.0719	-0.5628	0.0008
0.3025	-14.5425	-0.2702	1.4811	-0.1184	-1.0721	0.0016
0.4645	-16.6241	-0.2832	1.5402	-0.1311	-1.2823	0.0020
0.6343	-14.7427	-0.2203	1.1851	-0.1114	-1.0612	0.0019
0.8126	-8.8301	-0.1169	0.6247	-0.0649	-0.5824	0.0012
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Tetrachloroethylene + Cyclohexanone at 318.15 K						
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1478	-11.3214	-0.1355	0.9965	-0.0635	-0.6437	0.0007
0.3025	-17.6414	-0.2437	1.7215	-0.1048	-1.1745	0.0014

0.4645	-19.8626	-0.2587	1.8407	-0.1167	-1.3752	0.0018
0.6343	-17.8613	-0.2002	1.4449	-0.0974	-1.1684	0.0016
0.8126	-11.3702	-0.1022	0.7786	-0.0544	-0.6632	0.0010
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 4: The Figures of excess values of ultrasonic velocity (U^E), adiabatic compressibility ($\beta_{ad}{}^E$), enthalpy (H^E), Intermolecular free length ($L_f{}^E$), Molar volume ($V_m{}^E$) and Gibb's free energy (ΔG^E) for the binary liquid mixtures of tetrachloroethylene with cyclohexanone at 303.15 to 318.15K

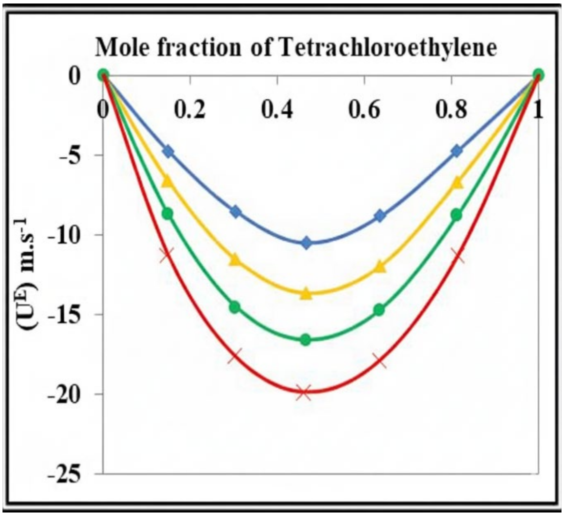

Fig. 1*:* Variation of excess Ultrasonic velocity

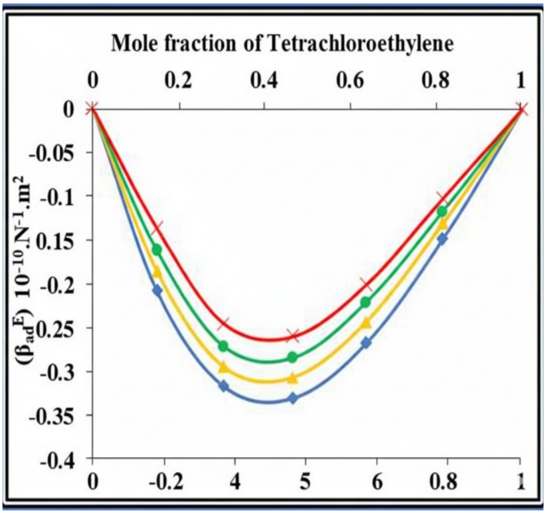

Fig. 2: Variation of excess adiabatic compressibility

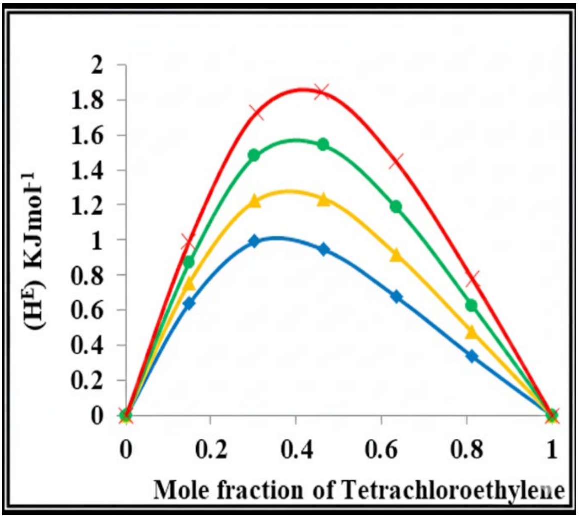

Fig. 3: Variation of excess enthalpy

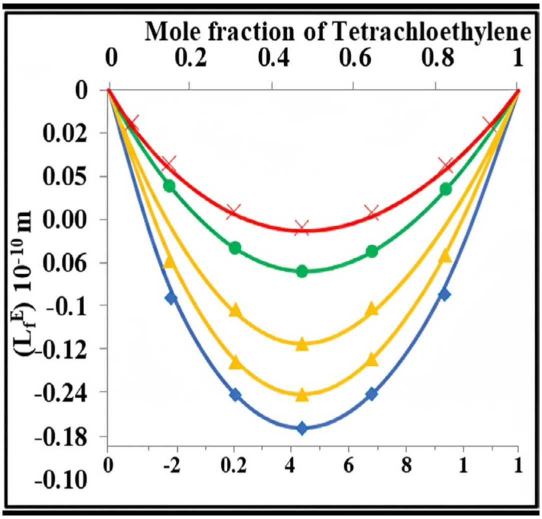

Fig. 4: Variation of excess free-length

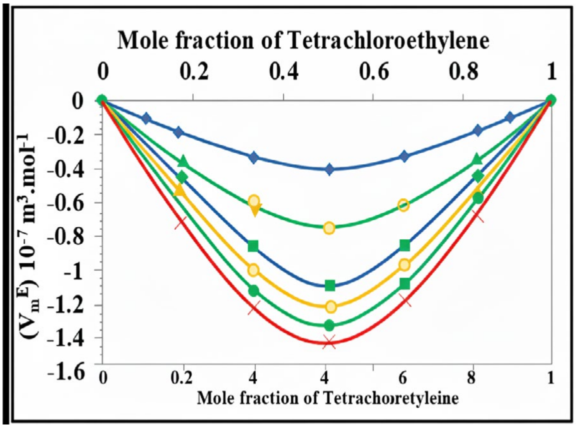

Fig. 5: Variation of excess Molar volume

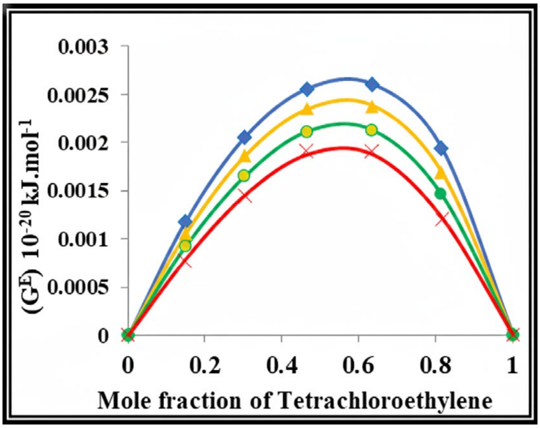

Fig. 6: Variation of excess Gibb's free energy

The data compiled in Table 1 summarize the relevant literature values used for comparison. Based on the experimentally measured density, viscosity, and ultrasonic velocity, the excess thermo-acoustic and thermodynamic parameters of the binary mixture of tetrachloroethylene and cyclohexanone were calculated over the entire mole-fraction range at different temperatures (Tables 2 and 3). The composition dependence of these parameters is illustrated in Figures 1–6 to facilitate clearer interpretation of molecular interactions.

Fig. 1 presents the variation of excess ultrasonic velocity (U^E). The values remain negative throughout the whole composition range and show a minimum near the equimolar region. This indicates that the mixture exhibits lower sound velocity than the corresponding ideal system, reflecting structural rearrangement and significant interaction between unlike molecules. The deviation from ideality suggests restricted molecular mobility due to dipole-induced dipole and dispersion interactions operating within the mixture(30).

Fig. 2 depicts the excess adiabatic compressibility ($\beta_{a_d}^E$), which is negative for all compositions. Negative $\beta_{a_d}^E$ values signify reduced compressibility compared to the ideal case, implying stronger cohesive forces and enhanced molecular packing. This behavior supports the presence of specific interactions, possibly involving weak hydrogen-bond-assisted attraction between the carbonyl oxygen of cyclohexanone and the chlorine atoms of tetrachloroethylene, along with dispersion contributions, as discussed in earlier studies (31-32).

Fig. 3 shows that the excess enthalpy (H^E) is positive across the entire mole-fraction range, indicating that the mixing process is endothermic. This suggests that interactions in the pure liquids are partially disrupted and replaced by comparatively weaker unlike-molecule interactions. The maximum near the equimolar composition corresponds to the region of greatest structural adjustment during mixing (33-34). As the proportion of tetrachloroethylene increases, dispersion forces become more prominent, reinforcing the contribution of weak dipolar interactions in the system(35-36).

Fig. 4 illustrates the variation of excess free length (L_f^E), which remains negative throughout, signifying decreased intermolecular free space and closer molecular approach(37). Similarly, Fig. 5 shows strongly negative excess molar volume (V_m^E), values, indicating volume contraction upon mixing. This contraction suggests efficient packing between molecules of different size and shape and supports the presence of hydrogen-bond-type associations along with the disruption of self-association in the pure components.

The magnitude of these effects decreases with increasing temperature, as thermal agitation tends to weaken intermolecular attractions(38–39).

Fig. 5 presents the variation of excess molar volume V_m^E with mole fraction of tetrachloroethylene (TCE). At lower concentrations of TCE, V_m^E exhibits small positive values, which suggest that the mixing process initially leads to slight expansion. This behavior can be attributed to weak dispersion forces and imperfect packing between unlike molecules. As the mole fraction of TCE increases, V_m^E gradually shifts to negative values, indicating volume contraction. Such contraction reflects stronger attractive interactions between the components, resulting in closer molecular approach and more compact structural arrangement. The transition from positive to negative values clearly points toward composition-dependent intermolecular interactions and improved packing efficiency at higher TCE content.

Fig. 6 shows the variation of excess Gibbs free energy of activation (ΔG^E) with composition and temperature. The observed increase in ΔG^E with rising mole fraction and temperature implies enhanced resistance to molecular flow, which is commonly associated with stronger associative interactions. This suggests that the mixture forms transient, structured arrangements due to intermolecular attractions(40). These findings are significant from an application standpoint, as tetrachloroethylene-based systems have been reported to aid in the extraction of organic sulfur compounds from coal, highlighting their potential usefulness in desulfurization technologies (41).

Table 5 presents the theoretically calculated values of ultrasonic velocity for the binary liquid mixtures over the complete mole-fraction range of Tetrachloroethylene at the selected temperatures. These values were evaluated using different theoretical approaches, namely the impedance relation, Nomoto's model, Junjie's theory, the ideal mixing rule, Rao's specific velocity relation, and the free-length theory. Each model is based on specific assumptions regarding molecular structure and interaction in liquid systems. The calculated results are compared with the experimental ultrasonic velocities to determine their reliability. The percentage deviations, whether positive or negative, indicate the strength and type of intermolecular interactions present. The model showing the least deviation is considered most suitable for explaining the acoustic behavior of the mixture.

Table 5: Ultrasonic velocity experimental and theoretical values at temperatures (303.15, 308.15, 313.15, and 318.15) K for the Tetrachloroethylene mole fraction with Cyclohexanone.

Mole Fraction(X)	**U_{EXP} ms^{-1}**	**U_J ms^{-1}**	**U_{NOM} ms^{-1}**	**U_{IMX} ms^{-1}**	**U_{RAO} ms^{-1}**	**U_{FLT} ms^{-1}**	**U_{IDR} ms^{-1}**
303.15 K							
0.0000	1388.79	1388.79	1388.79	1388.79	1388.79	1388.79	1388.79
0.1478	1329.65	1306.03	1323.74	1305.87	1550.88	1297.32	1306.19
0.3025	1272.54	1235.27	1260.76	1234.99	1624.03	1278.32	1235.16
0.4645	1212.24	1173.83	1199.81	1173.49	1595.10	1203.65	1173.44
0.6343	1148.24	1119.81	1140.85	1119.49	1467.91	1165.54	1119.30
0.8126	1089.35	1071.82	1083.86	1071.60	1270.18	1084.28	1071.43
1.0000	1028.80	1028.80	1028.80	1028.80	1028.80	1028.80	1028.80
308.15 K							
0.0000	1388.79	1370.58	1370.58	1370.58	1370.58	1370.58	1370.58
0.1478	1306.19	1287.24	1304.90	1287.43	1529.92	1304.30	1287.37

0.3025	1235.16	1215.94	1241.36	1216.22	1601.16	1273.54	1215.81
0.4645	1173.44	1154.02	1179.91	1154.29	1570.55	1202.27	1153.61
0.6343	1119.30	1099.56	1120.53	1099.77	1443.64	1142.22	1099.04
0.8126	1071.43	1051.17	1063.17	1051.28	1255.96	1087.12	1050.78
1.0000	1007.80	1007.80	1007.80	1007.80	1007.80	1007.80	1007.80
313.15 K							
0.0000	1353.72	1353.72	1353.72	1353.72	1353.72	1353.72	1353.72
0.1478	1292.35	1270.91	1288.37	1271.24	1507.82	1285.34	1271.14
0.3025	1234.34	1200.04	1225.17	1200.52	1577.33	1203.71	1200.04
0.4645	1173.84	1138.46	1164.06	1138.95	1547.84	1167.51	1138.18
0.6343	1112.75	1084.30	1105.02	1084.69	1422.75	1102.24	1083.88
0.8126	1052.69	1036.16	1048.01	1036.38	1224.89	1064.29	1035.82
1.0000	993.00	993.00	993.00	993.00	993.00	993.00	993.00
318.15 K							
0.0000	1343.59	1343.59	1343.59	1343.59	1343.59	1343.59	1343.59
0.1478	1272.35	1259.67	1277.30	1260.60	1485.23	1298.67	1260.35
0.3025	1212.65	1187.98	1213.22	1189.22	1554.45	1212.34	1188.49
0.4645	1154.67	1125.65	1151.31	1126.90	1525.98	1184.35	1125.84
0.6343	1094.39	1070.78	1091.54	1071.81	1402.59	1102.57	1070.72
0.8126	1035.38	1022.00	1033.87	1022.60	1214.23	1065.27	1021.87
1.0000	978.26	978.26	978.26	978.26	978.26	978.26	978.26

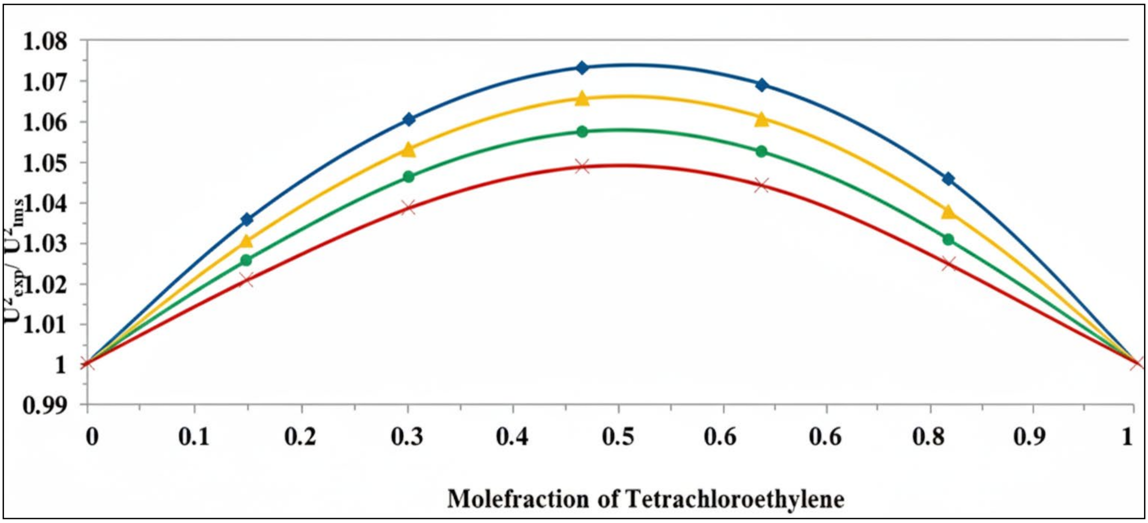

Fig. 7: Variaton of / with mole fraction of Tetrachloroethylene + Cyclohexanone

The comparative analysis of theoretical models shows that Rao's relation produces positive percentage deviations, while the other models result in negative deviations throughout the composition range. Among all the approaches considered, the free-length theory provides values that are closest to the experimentally measured ultrasonic velocities, indicating its greater reliability for representing this binary mixture.

The deviations observed between experimental and theoretical values clearly suggest non-ideal behavior of the system. The predominantly negative deviations obtained from most models point toward appreciable intermolecular attractions between the unlike molecules. Such behavior supports the existence of specific interactions, which may arise from dipole–dipole forces along with weak hydrogen-bond-type associations.

Fig. 7 presents a positive interaction parameter, further confirming the presence of molecular interactions within the mixture. In addition, the gradual decrease in the ratio / with increasing temperature indicates that the strength of interaction between the components diminishes at higher temperatures. This trend can be attributed to increased thermal agitation, which weakens cohesive forces and reduces the extent of association between the unlike molecules.

FT-IR Studies on Tetrachloroethylene with Cyclohexanone binary mixtures

The structural features of the solution and the nature of intermolecular interactions can be explored through spectroscopic methods such as FT-IR, which provide insight into how functional groups respond to their condensed-phase environment (42). In this study, FT-IR spectra were obtained for the cyclohexanone–tetrachloroethylene binary system at 298.15 K over the full range of compositions to examine the molecular interactions present in the mixture.

Figs. 8, 9, and 10 display the FT-IR spectra for pure tetrachloroethylene, the equimolar mixture of tetrachloroethylene and cyclohexanone (TCE + CYP = 1:1 ratio), and pure cyclohexanone, respectively. Cyclohexanone, being a ketone, exhibits characteristic absorption bands such as alkyl C–H stretching in the 2800–3000 cm^{-1} region, a strong C=O stretching band between 1670 and 1820 cm^{-1}, and a C–C stretching vibration near 1310 cm^{-1}.

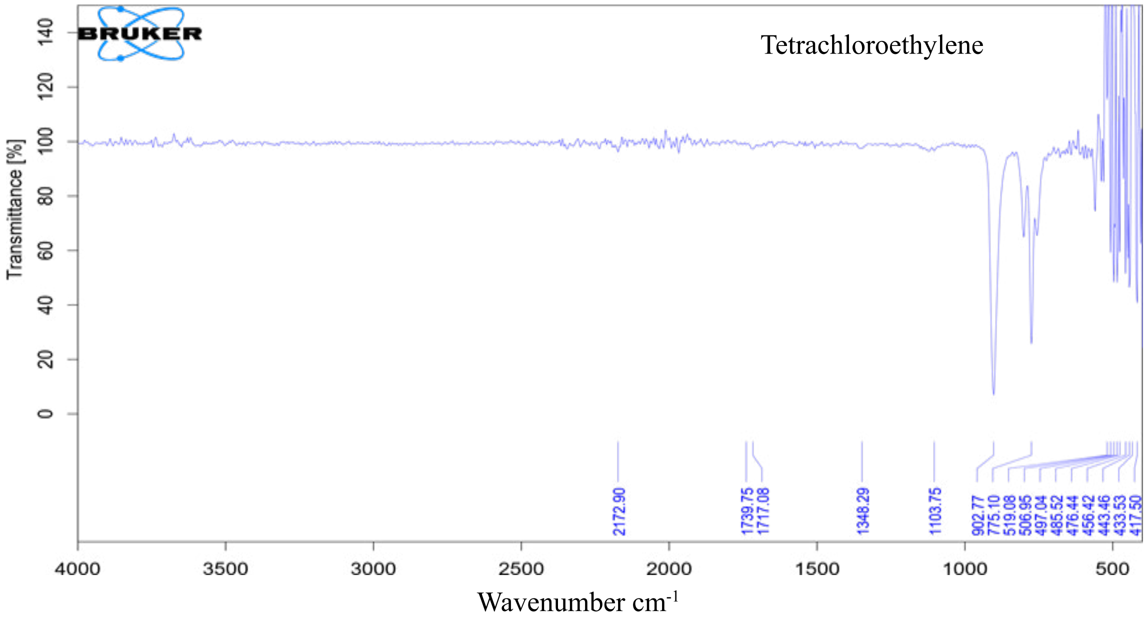

Fig. 8: FT-IR Spectrum of Tetrachloroethylene

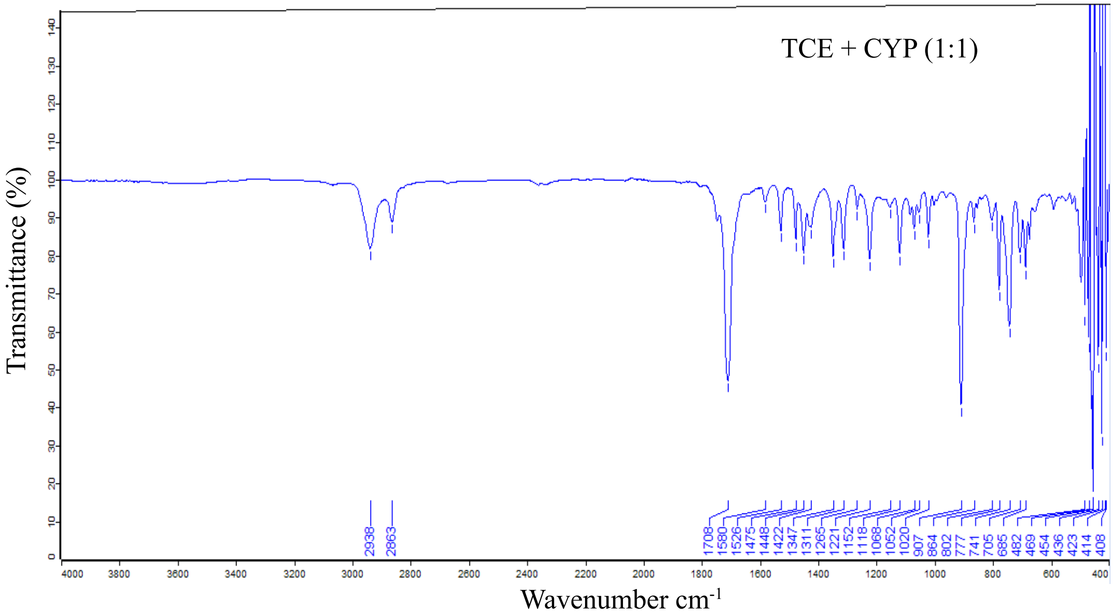

Fig. 9: FT-IR Spectrum of Tetrachloroethylene + Cyclohexanone (1:1)

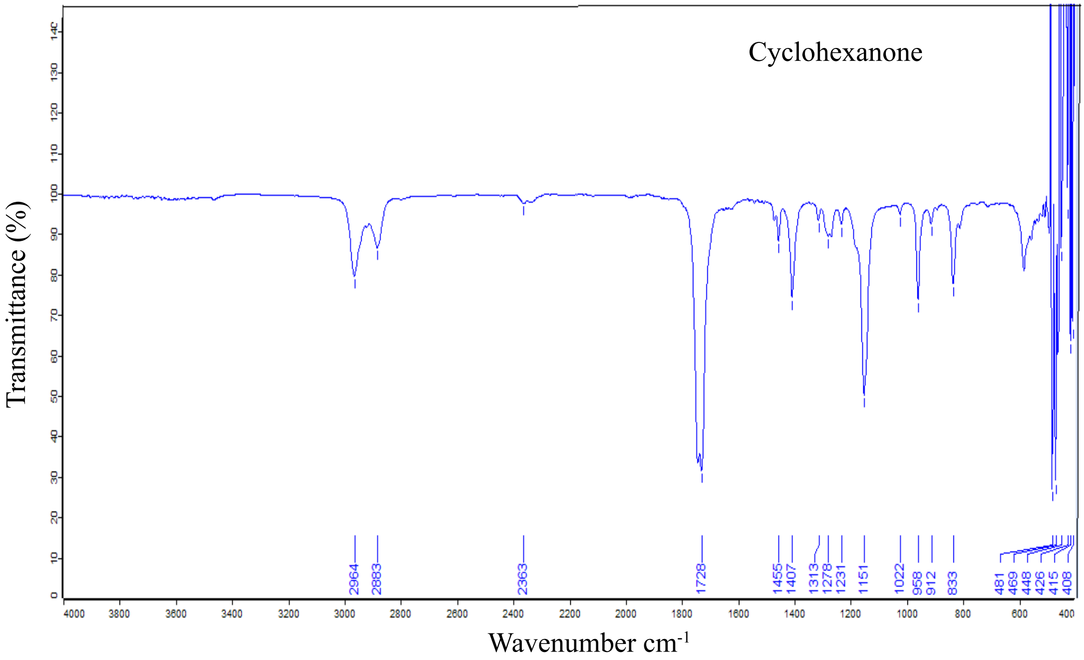

Fig. 10: FT-IR Spectrum of Cyclohexanone

The FT-IR spectrum of TCE shows a C=C bending vibration near 902.77 cm^{-1} and a C–Cl stretching band around 775.10 cm^{-1}. When tetrachloroethylene is mixed with cyclohexanone, the positions of these

IR bands shift progressively with composition, indicating changes in the molecular environment across the different mixtures.

The C=O stretching band shifts from its original position at 1728 cm^{-1}, with the largest change occurring at the equimolar mixture of the two liquids. This shift indicates the presence of strong interactions between tetrachloroethylene and cyclohexanone. The alteration in this key vibrational band suggests the formation of weak hydrogen-bond-type associations between the unlike molecules, as supported by theoretical predictions. The trends observed in the excess thermodynamic parameters, which point to significant intermolecular interactions, are further validated by the IR spectral evidence(43-48).

FUTURE DIRECTIONS

The present study on the binary mixture of Tetrachloroethylene and Cyclohexanone confirms significant intermolecular interactions through excess thermo-acoustic parameters, ultrasonic velocity models, and FT-IR analysis. To strengthen these findings, future work may extend measurements to slightly wider temperature and pressure ranges to better understand the thermal stability and structural variations of the system.

Detailed temperature-dependent FT-IR studies are suggested to quantitatively correlate shifts in the C=O stretching frequency with excess molar volume, compressibility, and Gibbs free energy. Application of Redlich–Kister polynomial fitting to the excess data would provide reliable interaction coefficients and improve agreement between experimental and theoretical models. Statistical deviation analysis of ultrasonic theories may also help identify the most suitable predictive model for this system.

Further extension of this work to ternary mixtures involving tetrachloroethylene, cyclohexanone, and an alcohol or other polar solvent would allow comparison of associative effects and interaction strength. Additionally, molecular dynamics or DFT calculations focused on these systems could provide microscopic insight into the experimentally observed negative excess properties and structural effects.

CONCLUSION

In this investigation, the nature of molecular interactions in the binary mixture of Tetrachloroethylene and Cyclohexanone was analyzed using acoustical, thermodynamic, theoretical, and spectroscopic methods.

The excess parameters - excess ultrasonic velocity (U^E), excess molar volume (V_m^E), excess adiabatic compressibility (β_{ad}^E), excess free length (L_f^E), excess enthalpy (H^E), and excess Gibbs free energy (ΔG^E) were calculated from experimentally measured ultrasonic velocity (u), density (ρ), and viscosity (η). Excess properties represent the deviation of real mixture behavior from ideal mixing. Therefore, they provide direct information about intermolecular interactions between unlike molecules.

The excess molar volume (V_m^E), shows a slight transition from positive to negative values with composition. A positive V_m^E generally indicates expansion due to weak interactions or structural loosening, while a negative V_m^E suggests volume contraction caused by closer molecular packing. The observed transition implies that, at certain compositions, attractive forces between tetrachloroethylene and cyclohexanone molecules become significant enough to cause structural rearrangement and tighter packing. This contraction behavior is commonly associated with dipole–dipole interactions and weak hydrogen-bond-type associations involving the carbonyl (C=O) group of cyclohexanone.

Similarly, the trends in excess compressibility (β_{ad}^{E}) and excess free length (L_f^{E}) support the presence of attractive interactions. A decrease in compressibility and free length indicates that molecules are brought closer together due to intermolecular attractions. The negative values of excess Gibbs free energy (ΔG^{E}) further confirm that the mixing process is thermodynamically favorable and dominated by specific interactions rather than random mixing.

Among the theoretical models used to predict ultrasonic velocity, the free-length theory shows the closest agreement with experimental values. This suggests that the intermolecular free space (free length) plays a major role in determining the acoustical behavior of this system. The good correlation validates the applicability of this theory for describing molecular interactions in this binary mixture.

FT-IR spectral analysis provides additional confirmation of these interactions. In pure cyclohexanone, a strong absorption band appears at 1710–1725 cm^{-1} due to C=O stretching vibration of the carbonyl group. Pure tetrachloroethylene exhibits characteristic C–Cl stretching bands in the 600–900 cm^{-1} region. In the equimolar mixture, the C=O stretching band remains present but shows a slight shift and broadening. Such spectral changes indicate that the carbonyl group experiences a modified local environment due to interaction with tetrachloroethylene molecules.

Importantly, no new peaks appear in the mixture spectrum, and all characteristic bands of the individual components are retained. This confirms that no new chemical compound is formed. Therefore, the observed changes arise from physical interactions—mainly dipole–dipole attractions and weak dispersion forces—rather than chemical reactions.

Overall, the combined acoustical, thermodynamic, theoretical, and FT-IR results consistently demonstrate significant intermolecular attractions in the binary mixture, supporting the proposed interpretation of molecular interaction mechanisms.

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