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Thermo-Acoustic Parameter Analysis of Binary Liquid Mixtures of 2-Methyl Cyclohexanone with Water/1-Propanol and 2-Propanol: Investigating Intermolecular Interactions at Various Temperatures

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Abstract

Conducted as a comprehensive investigation, this study delves into the intricate realm of intermolecular interactions within binary liquid mixtures, specifically focusing on the pairing of 2-methylcyclohexanone with water/1-propanol and 2-propanol. An exploration of various thermo-acoustic parameters has been undertaken to unravel the nuanced nature of these interactions.The experimental facet of this study involved meticulous measurements of density (ρ) and speed of sound (U) conducted over a temperature range spanning from 303.15 to 313.15 K, with data points captured at 5 K intervals. These measurements took place within the confines of ambient atmospheric pressure conditions, ensuring a controlled experimental environment.Harnessing the wealth of experimentally determined data, this investigation strategically calculated two pivotal thermo-acoustic parameters: excess isentropic compressibility ((K_S^E) and excess molar volume (V_m^E). These parameters serve as indispensable tools, providing invaluable insights into the dynamic behavior exhibited by the

liquid mixtures under scrutiny. The calculated excess functions were meticulously correlated using a reduced Redlich-Kister polynomial equation, amplifying the depth of our understanding regarding the molecular interactions at play. The results obtained from this meticulous analysis cast a spotlight on the robustness of structural molecular interactions among the components within the binary mixtures. Notably, intriguing patterns emerged when scrutinizing different compositions, revealing a discernible trend. The 2-methylcyclohexanone + 2-propanol mixture exhibited notably stronger interactions when juxtaposed against other composite mixtures, highlighting the distinctive strength and intricacy characterizing this specific pairing.

Emerging Trends and Future Directions:

As we navigate through the findings of this investigation, it sets the stage for contemplating emerging trends and future directions in the realm of intermolecular interactions within binary liquid mixtures. The highlighted strength of structural molecular interactions paves the way for potential applications in fields ranging from industrial processes to pharmaceutical formulations. Future explorations may delve deeper into the specific mechanisms underpinning the observed trends, opening avenues for tailored applications and the development of novel mixtures with enhanced properties. Additionally, the nuanced understanding gained from this study provides a solid foundation for exploring similar interactions in diverse systems, offering opportunities for cross-disciplinary investigations and the discovery of new frontiers in molecular science.

Keywords: Redlich-kister equations, reduced Redlich kister equations, partial isentropic compressibilities, partial molar volumes etc.

1 Introduction

Examining fundamental thermodynamic characteristics, specifically density and the speed of sound, in binary systems is pivotal for numerous industrial applications and contemporary research. The goal of this study is to gain insights into the intricate molecular interactions within binary systems by analyzing these fundamental characteristics across various temperature intervals under standard atmospheric pressure.

Deriving excess thermodynamic acoustic parameters by analyzing these fundamental characteristics provides valuable information about the nature of specific and non-specific interactions. These parameters encompass details such as interaction strength, the presence of dipoles, and the steric behavior of molecules within composite mixtures. Previous pioneers in the field extensively explored these intermolecular interactions, considering excess thermodynamic acoustic parameters.

In this experimental setup, two isomers of propanol and water[1] were independently combined with 2-methylcyclohexanone (2MCH). Notably, 2MCH, with its steric chair flip cycloalkane structure, is widely used as a solvent in both industrial and pharmaceutical sectors. Previous research delved into the unique combinations of the aromatic aniline group with the chiral cyclohexanone group[2].

Several pioneers[3-6] eclectically researched the combination of aromatic aniline group with chiral cyclohexanone group.

This study specifically investigates multi-component liquid mixtures involving water (W), 1-propanol (1P), and 2-propanol (2P) when combined with 2MCH. The experiments were conducted at regular temperature intervals ranging from 303.15 K to 313.15 K, maintaining constant ambient atmospheric pressure conditions. To assess molecular interactions effectively, excess values such as excess volume (V_m^E) and excess isentropic compressibility ($K_{s,m}^E$) were calculated. These values were then fitted to a non-linear polynomial regression equation known as the Redlich-Kister (RK) equation, which is of the 4th order[7].

It is important to note that the combination of the aromatic aniline group with the methyl group of cyclohexanone exhibits high reactivity at low concentrations, which can occasionally lead to specific interaction results that may be misleading. To provide a more accurate depiction of intermolecular hydrogen bonding, the Reduced Redlich-Kister (RRK)[8,9] non-linear polynomial regression equation was employed. Additionally, understanding the extent of solvation behavior within composite mixtures was sought by determining partial molar volumes and partial isentropic compressibilities. These findings were then evaluated in terms of the intermolecular interactions occurring between the component molecules.

2 Material and methods

2.1 Specimen extraction

In Table-1, the present sequence illustrates the provenance, CAS number, purity, and further purification

under chromatography of water, 1-propanol, 2-propanol, and 2-methylcyclohexanone (2MCH). The drying methods for these substances have also been provided[10]. The chemical data inventories for propanol isomers and 2MCH are archived in Table 1. Additionally, Table 2 presents the density and speed of sound of pure fluids, such as water, 1-propanol, 2-propanol, and 2-methoxycyclohexanone, along with relevant citations.[12]

Table 1

Specification of Source, CAS Number, Mass Fraction Purity and Further Purification

Name of the chemical	Source	CAS Number	Mass fraction purity	Further purification methods
Water	Double Distillation Method	7732-18-5	>99.99%	----
1-propanol	HiMedia Laboratories, India	71-23-8	>98.00%	*GLPC
2-propanol	HiMedia Laboratories, India	67-63-0	>98.00%	*GLPC
2MCH	HiMedia Laboratories, India	583-60-8	>99.70%	*GLPC

*Gas-Liquid partition chromatography carried through inert gas Ar.

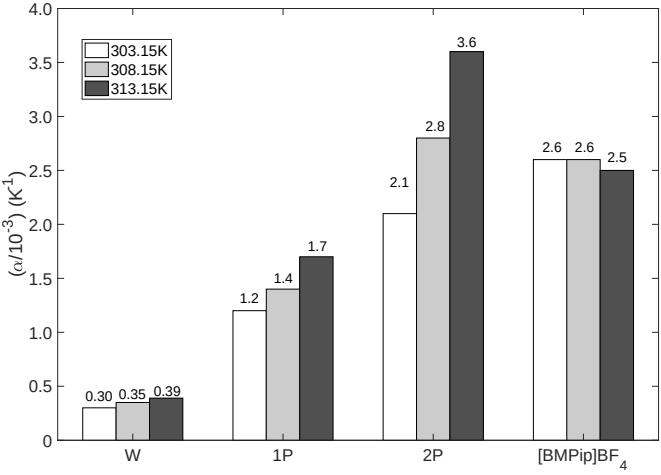
Table 2

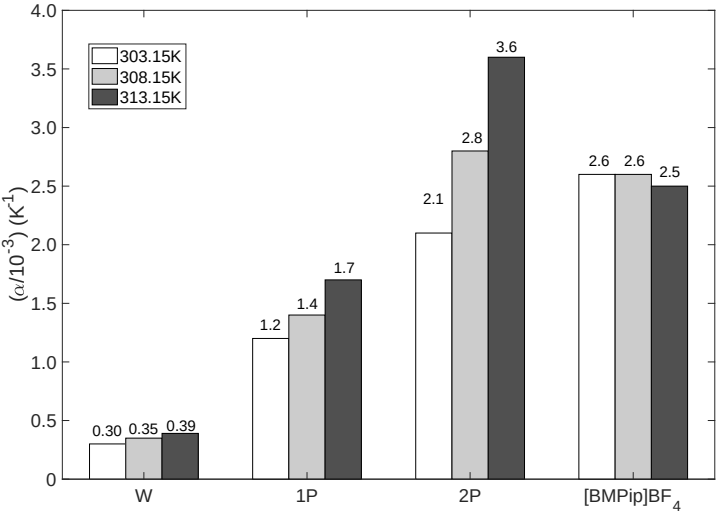
Physical properties of pure component water, 1-propanol, 2-propanol and 2-methoxy cyclohexanone with literature at specific temperatures

Sample	Parameter	Expt./Lit.	Temperatures		
			303.15K	308.15K	313.15K
2-propanol	ρ (kg. m^{-3})	Expt.	782.00	772.50	760.20
	ρ (kg. m^{-3})	Lit.	781.50[a]	772.00[a]	760.10[a]
	ρ (kg. m^{-3})	Lit.	776.85[e]	772.49[e]	768.05[e]
	U (m.s^{-1})	Expt.	1122.40	1106.00	1088.64
	U (m.s^{-1})	Lit.	1122.20[a]	1106.20[a]	1088.80[a]
	U (m.s^{-1})	Lit.	1121.43[e]	1103.94[e]	1086.62[e]
1-propanol	ρ (kg. m^{-3})	Expt.	798.52	793.30	787.02
	ρ (kg. m^{-3})	Lit.	798.50[d]	793.30[d]	786.90[d]
	ρ (kg. m^{-3})	Lit.	775.97[e]	791.89[e]	787.77[e]
	U (m.s^{-1})	Expt.	1189.24	1171.74	1150.10
	U (m.s^{-1})	Lit.	1189.20[d]	1171.80[d]	1150.00[d]
	U (m.s^{-1})	Lit.	1189.26[e]	1172.37[e]	1155.53[e]
water	ρ (kg. m^{-3})	Expt.	995.64	994.04	992.21
	ρ (kg. m^{-3})	Lit.	995.67[b]	994.04[b]	992.23[b]
	ρ (kg. m^{-3})	Lit.	995.70[c]	994.03[c]	992.16[c]
	U (m.s^{-1})	Expt.	1509.12	1519.82	1528.90
	U (m.s^{-1})	Lit.	1509.25[b]	1519.82[b]	1528.89[b]
	U (m.s^{-1})	Lit.	1509.25[c]	1519.82[c]	1528.89[c]
2MCH	ρ (kg. m^{-3})	Expt.	920.80	911.22	907.45
	ρ (kg. m^{-3})	Lit.	920.84[d]	911.20[d]	907.44[d]
	U (m.s^{-1})	Expt.	1346.00	1324.30	1303.20
	U (m.s^{-1})	Lit.	1346.00[d]	1324.20[d]	1303.8[d]

*The calibrated uncertainties are $U_c(\rho)$=0.038 kg.m^{-3}, $U_c(U)$=0.416m.sec^{-1}, $U_c(x_1)$=0.000027, $U_c(T)$=0.01K are carried at ambient atmospheric pressure references [a][12], [b][12],

[c][5], [d][2],





2.2 Detection Methods

The prepared binary fluids and pure fluids were dispensed into vials. To prevent evaporation and the adsorption of atmospheric moisture, these vials were sealed with airtight lids. The fluids were weighed using a mass analytical balance (Mettler Toledo) with an accuracy of ±10-11 kg. Consequently, the uncertainty in measuring the final mole fraction for binary fluids should be less than ±0.0001.

Binary fluids of systems like 2MCH+Water(W), 2MCH+1-Propanol(1P), and 2MCH+2-Propanol(2P) were prepared at specified concentrations. The mole fractions of these systems were varied in 12 subsequent values, ensuring that the solvation concentration ranges from 0 to 1. The temperature-dependent thermophysical features of density (ρ) were calibrated using a vibrating-tube digital density meter. The speed of sound (U) was obtained with a sound analyzer within temperature ranges from 303.15K, 308.15K, and 313.15K over ambient atmospheric pressure.

These instruments were kept in a temperature bath with a tunable set of constant temperature ranges. The temperature bath was controlled through an incorporated peltier thermostat with an accuracy of ±0.01K. Consequently, the uncertainty in measuring the experimental density (ρ) and speed of sound (U) should be less than or equal to 0.01 $kg.m^{-3}$ and 0.5$m.s^{-1}$, respectively.[13-16]

2.3 Theory

The Experimentally extracted were the density (ρ) and speed of sound (U) for binary fluids of 2MCH+W, 2MCH+1P, and 2MCH+2P within temperature ranges 303.15K, 308.15K, and 313.15K. The variations of these parameters are illustrated in Figures 1(a) & 1(b), depicting a non-linear trend. The

observed features of a non-linear increasing trend suggest the existence of molecular interactions between the fluids[16]. Furthermore, these non-linear trends decrease as the temperature increases.

Excess thermodynamic acoustic parameters such as V_m^E and K_s^E for binary fluids have been estimated and documented in several peer-reviewed journals[17–20]. The eventual general expression was...

$$Y^E = Y^r - Y^{id} \quad ---- \quad (1)$$

Here $Y^E = V_m^E, K_s^E$ and Y^r {=V_m(molar volume), $K_{s,m}$ (molar isentropic compressibility)} are the real value of fluids. And, the ideal component of thermodynamic acoustic parameters for molar volume stands for

$$V^{id} = x_1 V_1 + (1 - x_1) V_2 \quad ---- \quad (2)$$

Here, x_1 is the molefraction of component 2MCH (1) with respect to W/1P/2P(2). V_1 and V_2 are the pure acoustic molar values of 2MCH(1) and W/1P/2P(2) respectively. The isentropic compressibility K_s was calculated from the equation

$$K_s = \frac{1}{\rho U^2} \quad ---- \quad (3)$$

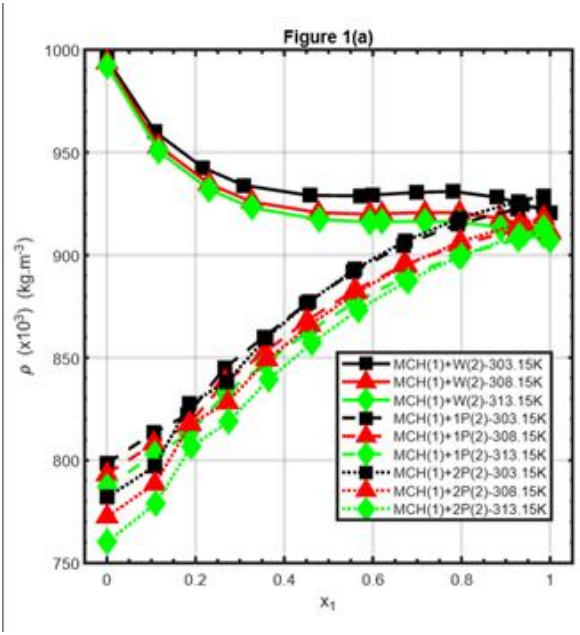
3.1 Redlich-Kister Polynomial Analysis

The conventional non-lineal curve fitting strategy for attributes of binary fluids pertains Redlich-Kister polynomial regression coefficients.

$$Y_{RK}^{E} = \mathrm{x}_1(1-\mathrm{x}_1)\Sigma_{p=0}^{p=n} A_{p,T}(2x_i-1)^p ----- (4)$$

Here, (Y_{RK}^{E}) means excess thermo dynamic feature which contain any value (i.e, V_m^E, $K_{s,m}^E$) has been taken. The standard deviation was also calibrated for the consequence.

$$\sigma(Y_{RK}^{E}) = \sqrt{\sum_{i=1}^{i=n} \frac{\left(Y_{i,exp} - Y_{i,cal}\right)^2}{m-n}} ----- (5)$$



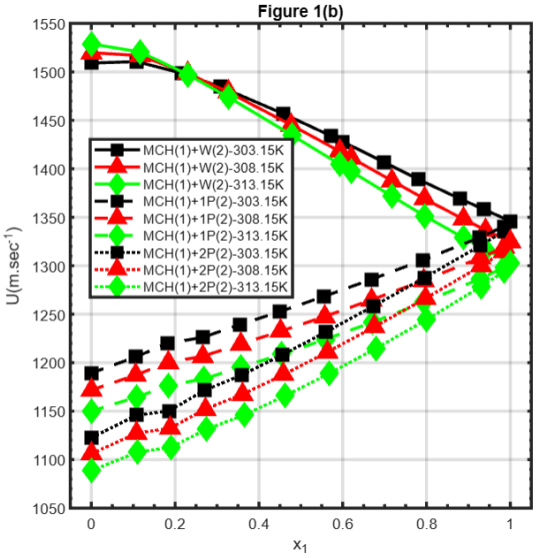
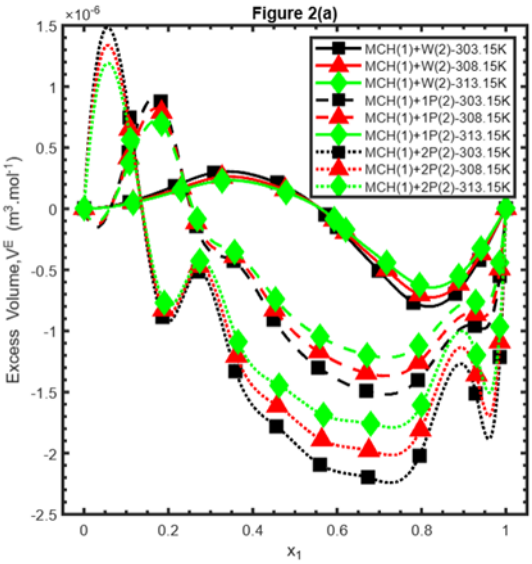


Fig. 1 Plot of thermo physical features versus mole fraction (a) density (b) speed of sound.

Where *m* stands for the number of experimental values and n stands for the adjustable parameter. These excess values are examined with Redlich-Kister polynomial non-linear regression coefficients. And these values of $A_{i,T}$(i=0,1,2,3) are determined along with standard deviation for the experimental values. The Table 3 catalogued the whole values of all composites. The abnormality of thermodynamic acoustic excess parameters of V_m^E, K_s^E are portrayed in Figure 2(a) & 2(b) respectively. Due to thermal agitations of all fluids, temperature rise ushers to descend the excess parameters. The abnormality of excess molar volume at all temperatures has been illustrated in Figure 2(a) over an entire concentration for

all composites[23,24]. The values of V_m^E are attributes positive or small negative for high concentrations of Water(W), 1-propanol(1P) & 2-propanol(2P) and the trend turns to negative during the increasing concentration of 2MCH in the respective composites.



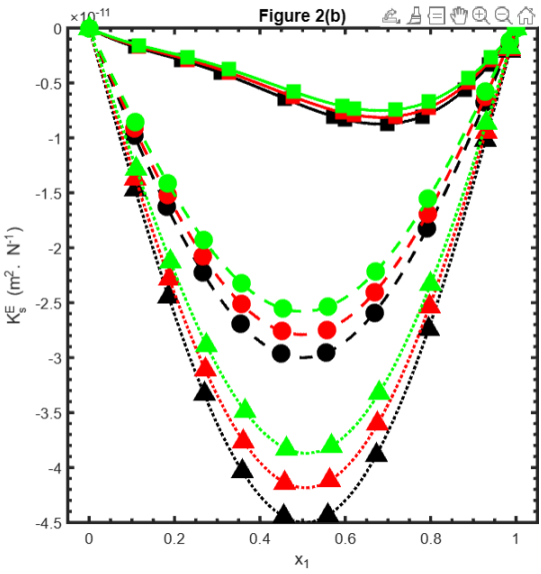


Fig. 2 Plot of excess thermo physical features versus molefraction (a) Excess molar Volume (b) Excess isentropic compressibility.

The negative value of excess molar volume V_m^E is greater in 2MCH + 2P compared to the other fluids such as 2MCH + 1P & 2MCH + W. This distinction is clearly visible in Figure 2(a). The negative sign of V_m^E indicates the formation of H-bonds, which are stronger at higher concentrations and weaker at lower concentrations of composites. Additionally, the formation of H-bonds is very weak at high concentrations of W, 1P, and 2P.

The negative value of excess molar volume K_s^E is greater in 2MCH + 2P compared to the other fluids such as 2MCH + 1P & 2MCH + W. This distinction is clearly visible

in Figure 2(b). The abnormal sign of K_S^E plays a vital role in assessing the compactness due to molecular interactions in multi-component mixtures through electric charge transfer, dipole-dipole interactions, and dipole-induced dipole interactions between bonds of successive constituent elements. It also suggests interstitial accommodation and oriental ordering leading to a more compact structure, enhancing K_S^E to negative values. Fort and Moore indicated that binary fluids with distinct molecular sizes and shapes mix well, thereby reducing the volume, causing K_S^E values to be negative. The K_S^E value of negativity was greater in 2MCH + 2P compared to the other composites of 2MCH + 1P & 2MCH + W, respectively [25]. This also clearly distinguishes greater steric hindrance to the formation of hydrogen bonds in the respective composites. The sign of V_m^E and K_S^E values indicates the strength of intermolecular interactions as 2MCH(1) + 2P(2) > 2MCH(1) + 1P(2) > 2MCH(1) + W(2).

Table 3

Coefficients of redlich-kister equation parameters and standard deviation for excess molar quantities at different temperatures.

Combination	T/K	Redlich-kister equation coefficients				error
		$A_{0,T}$	$A_{1,T}$	$A_{2,T}$	$A_{3,T}$	$\sigma(Y_{RK}^E)$
		V_m^E (10^{-6} $m^3.mol^{-1}$)				
	303.15	0.5327	-4.2470	-5.8506	-0.6545	0.0515

2MCH(1)+W(2)	308.15	0.4656	-3.7304	-5.3870	-0.8142	0.0387
	313.15	0.4131	-3.3125	-4.7867	-0.7266	0.0346
			$K_{s,m}^{E}$ (10^{-16} m^2 .N^{-1})			
	303.15	-28.2441	-30.2307	-12.1652	11.9465	1.64E-07
2MCH(1)+W(2)	308.15	-26.2670	-28.1145	-11.3136	11.1103	9.6E-08
	313.15	-24.2900	-25.9983	-10.4620	10.2740	4.8E-08
			V_m^{E} (10^{-6} m^3.mol^{-1})			
2MCH(1)+1P(2)	303.15	-3.9104	-4.4891	-0..9130	-13.4118	0.1061
	308.15	-3..5707	-4.3093	-0.5238	-11.4291	0.0904
	313.15	-3.1717	-4.0172	-0.3780	-9.9104	0.0700
			$K_{s,m}^{E}$ (10^{-16} m^2 .N^{-1})			

	303.15	-119.8354	0.2754	26.2862	-0.7409	0.0033
2MCH(1)+1P(2)	308.15	-111.4476	0.2426	24.4500	-0.6966	0.0031
	313.15	-103.0598	0.2279	22.6140	-0.6526	0.0028
		V_m^E (10^{-6} m^3.mol^{-1})				
	303.15	-6.7555	-3.9748	-3.2495	-21.0423	0.4308
2MCH(1)+2P(2)	308.15	-6.0808	-3.5512	-2.8211	-19.1251	0.4070
	313.15	-5.3949	-3.1224	-2.4302	-17.2252	0.3850
		$K_{s,m}^E$ (10^{-16} m^2 .N^{-1})				
	303.15	-179.7309	-4.1987	39.3579	0.5606	0.0051
2MCH(1)+2P(2)	308.15	-167.	-5.0602	36.5696	0.9367	0.0047

	1383				
31	-154.5382	-6.2093	33.757	1.4204	0.0043
3.15					

***The calibrated uncertainties are $U_c(V_m^E)$=0.00012x10^{-6}m^3.mol^{-1}, $U_c(K_{s,m}^E)$=3x10^{-18}m^2.N^{-1} are carried at ambient atmospheric pressure.*

3.2 Reduced Redlich-Kister Polynomial Analysis

The unavoidable Redlich-Kister approach sporadically misguides dissimilar composites, deceiving interactions of molecules at low concentration regions in composites. Consequently, Desnoyers[26] suggested a contemporary and befitting Reduced Redlich-Kister (RRK) polynomial analysis to address more specific features in composites[27,28].

Applying the reduced function on V_m^E and $K_{s,m}^E$, the graphs of Figure 2(a) & 2(b) transform into Figure 3(a) & 3(b), respectively. The abnormality of $Q_{V_m^E,T}(x_1)$ at all temperatures is illustrated in Figure 3(a) over an entire concentration for all composites. This evidently distinguishes that hydrophobic interactions are present and stronger in the region of higher concentrations. Additionally, hydrophobic interactions are very weak at high concentrations of W, 1P & 2P. The order of interactions in terms of values is 2MCH(1)+2P(2) > 2MCH(1)+1P(2) > 2MCH(1)+W(2).

In the present scenario, the reduced functions values $Q_{K_S^E,T}(x_1)$ are higher on the W/1P/2P side and lower on the 2MCH side. This is clearly visible in Figure 4(b), for the replicated sequence of $Q_{K_S^E,T}(x_1)$. This result indicates that

composites are less compressible than the corresponding ideal mixtures, strongly suggesting that strong interactions occur in these composites. It also clearly indicates that the 2P molecules are more sterically hindered in 2MCH molecules than the rest of the two binary fluids.

$$Q_{Y^E_{RRK}}(x_1) = \frac{Y^E_{RK}(x_1)}{x_1(1-x_1)} - - - - (10)$$

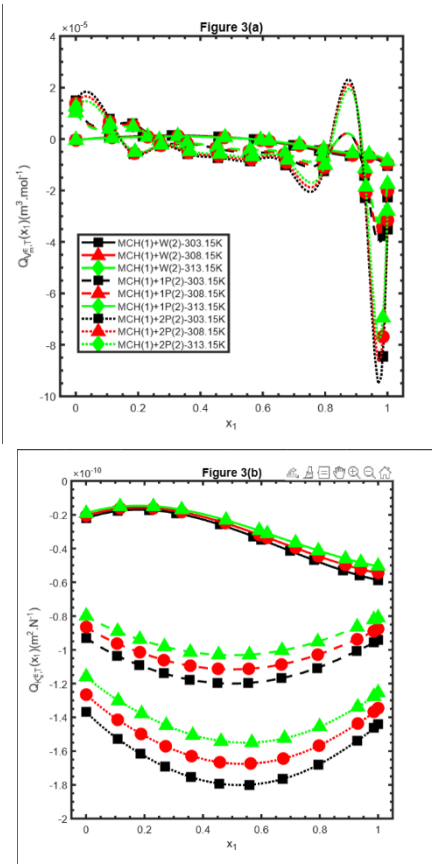
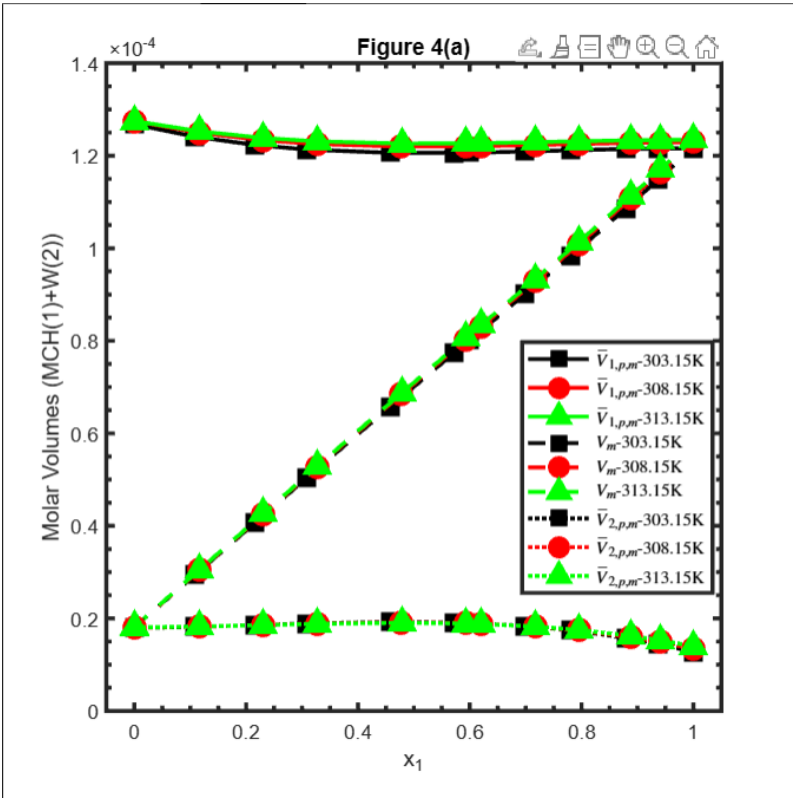


Fig. 3 Plot of reduced excess thermo physical features versus molefraction (a) Reduced excess molar Volume (b)Reduced excess molar isentropic compressibility.



3.3 Partial molar volumes and partial molar isentropic compressibilities

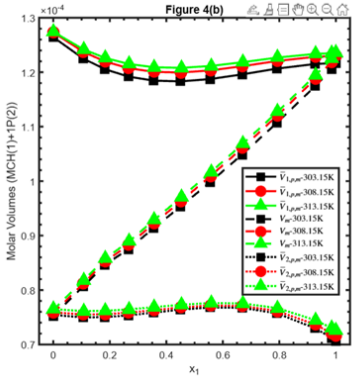
The RRK functions of $Q_{V_m^E,T}(x_1)$ and $Q_{K_{s,m}^E,T}(x_1)$ at infinite dilution over a constant temperature and pressure was an addition tool to represents partial molar volumes and partial

isentropic compressibilities at infinite dilutions[29]. The above extrapolation expression (8) has modified as

$$Q_{V_m^E}(x_1 = 0) = A_{0,T} - A_{1,T} + A_{2,T} - A_{3,T} = \bar{V}_{1,p,m}^{E,\infty} = \bar{V}_{1,p,m}^{\infty} - V_{1,m} \quad ----(11)$$

$$Q_{V_m^E}(x_1 = 1) = A_{0,T} + A_{1,T} + A_{2,T} + A_{3,T} = \bar{V}_{2,p,m}^{E,\infty} = \bar{V}_{2,p,m}^{\infty} - V_{2,m} \quad ----(12)$$

$\bar{V}_{1,p,m}^{E,\infty}$ *and* $\bar{V}_{2,p,m}^{E,\infty}$ are excess partial molar volumes two pure components at infinite dilutions. $\bar{V}_{1,p,m}^{\infty}$ *and* $\bar{V}_{2,p,m}^{\infty}$ are partial molar volumes at infinite dilutions. $V_{1,m}$ and $V_{2,m}$ are pure molar volumes of two components 2MCH and W,1P & 2P. Similarly, the equation analogy is also true for partial isentropic compressibilities. But, the real-time analysis of partial molar volumes and partial isentropic compressibilities over a molefraction concentration at constant pressure and temperature can be evaluated from the differential equation is



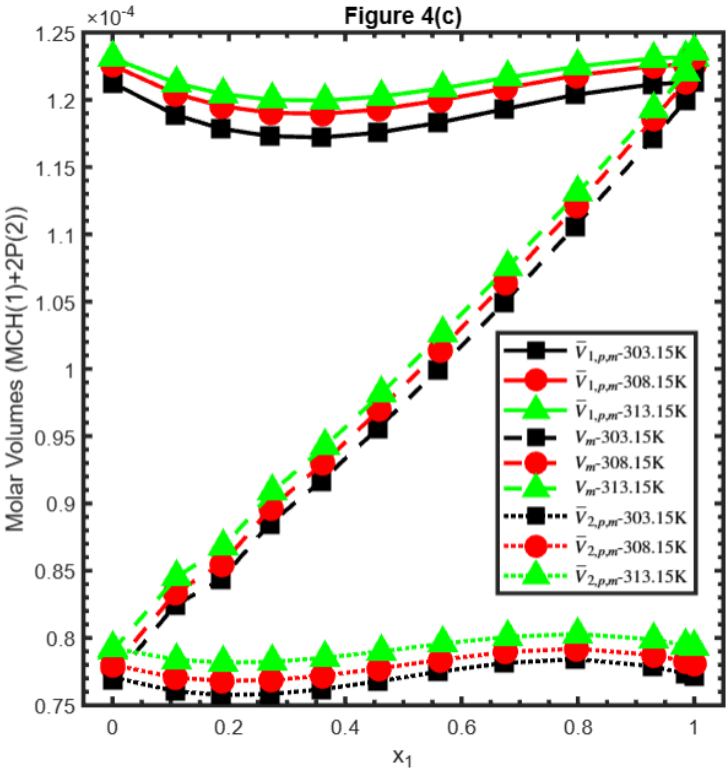
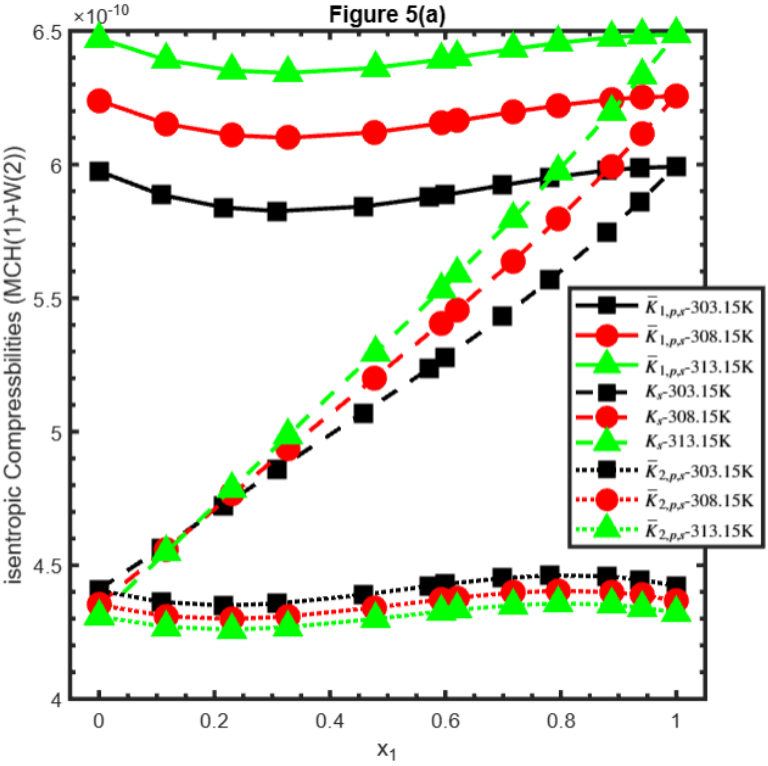


Fig. 4 Plot of partial molar volume against molefraction and temperature for the solution (a)2MCH(1)+W(2) (b)2MCH(1)+1P(2) (c)2MCH(1)+2P(2)



$$\bar{V}_{i,p,m} = V_m(x_i) - x_j \left(\frac{\partial V_m(x_j)}{\partial x_j}\right)_{T,P} \quad ----(13)$$

$$\bar{K}_{i,p,s} = K_s(x_i) - x_j \left(\frac{\partial K_s(x_j)}{\partial x_j}\right)_{T,P} \quad ----(14)$$

Here x_i and x_j are the mole fractions of two components in the composite ($i=1,2$ & $j=i-1$).

Analyzing intermolecular interactions within the composites involves a nuanced consideration of the packing efficiency of molecules, employing critical parameters such as partial molar volumes and partial isentropic compressibilities. The pivotal role played by the partial molar volumes $\bar{V}_{1,p,m} and\ \bar{V}_{2,p,m}$ in binary fluids cannot be overstated[30], given that the domain influence of components within the mixture undergoes dynamic changes contingent on composition concentration and temperature variations. Illustrating this scenario, Figure 4(a), 4(b), and 4(c) depict the partial molar volumes of components 2MCH+2P, 2MCH+1P, and 2MCH+W across a spectrum of temperatures.[30]

Each figure encapsulates a scaffolded Z symbol graph adorned with three distinct colored curves $\bar{V}_{1,p,m}, V_m\ and\ \bar{V}_{2,p,m}$. Notably, the partial molar volumes $\bar{V}_{1,p,m} and\ \bar{V}_{2,p,m}$ for all combinations are consistently lower than their individual values in a pure state. This discrepancy elucidates the diminishing domain influence of individual components as concentrations decrease. The abnormality is scrutinized across constant temperature intervals, unequivocally pointing towards the existence of solute-solvent interactions between dissimilar molecules. Thus, the representation in Figure 4(a), 4(b), and 4(c) underscores that the effect of domain influence on volume is less pronounced for 2MCH+2P compared to the other composites of 2MCH+1P & 2MCH+W, respectively, signifying heightened solute-solvent interactions.

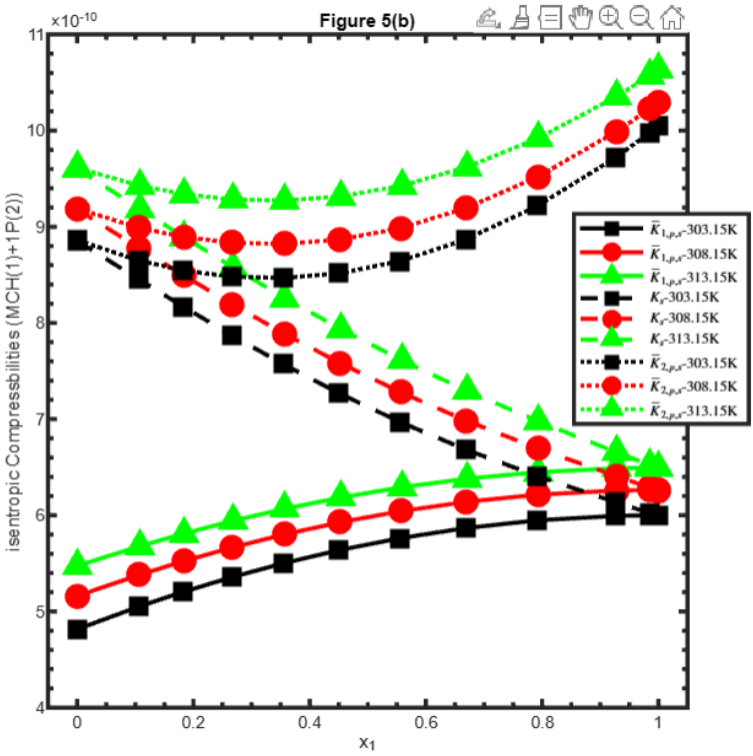


Figure 5(b)
×10-10
isentropic Compressbilities (MCH(1)+1P(2))
x1
0
0.2
0.4
0.6
0.8
1
4
5
6
7
8
9
10
11
$\bar{K}_{1,p,s}$-303.15K
$\bar{K}_{1,p,s}$-308.15K
$\bar{K}_{1,p,s}$-313.15K
K_ϕ-303.15K
K_ϕ-308.15K
K_ϕ-313.15K
$\bar{K}_{2,p,s}$-303.15K
$\bar{K}_{2,p,s}$-308.15K
$\bar{K}_{2,p,s}$-313.15K

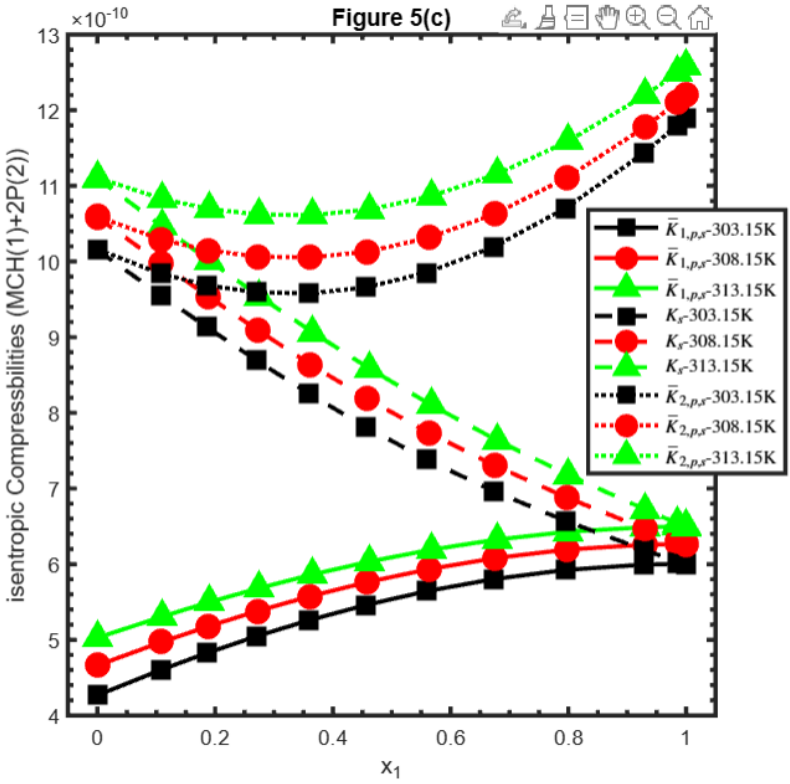


Fig. 5 Plot of partial molar isentropic compressibilities against molefraction and temperature for the solution (a)2MCH(1)+W(2) (b)2MCH(1)+1P(2) (c)2MCH(1)+2P(2).

Turning attention to the partial isentropic compressibilities $\bar{K}_{1,p,s}$ and $\bar{K}_{2,p,s}$, their indispensable role in binary mixtures cannot be understated[31], given that the geometrical influence of components evolves with changing

composition concentration and temperature. Figure 5(a), 5(b), and 5(c) encapsulate the partial isentropic compressibilities of components 2MCH+W, 2MCH+1P, and 2MCH+2P, respectively.

In each figure, a meticulously scaffolded Z symbol graph hosts three distinct colored curves $\overline{K}_{1,p,s}, K_s$ and $\overline{K}_{2,p,s}$. The higher values of partial isentropic compressibilities $\overline{K}_{1,p,s}$ and $\overline{K}_{2,p,s}$ for the combination 2MCH+2P, compared to 2MCH+1P & 2MCH+W, clearly signify an increased breaking of dipole inclusions between molecules. This emphasizes that the effect of geometrical influence is less pronounced for 2MCH+W when contrasted with the other composites of 2MCH+1P & 2MCH+2P, suggesting a higher degree of molecular interaction complexity within 2MCH+2P.[31]

4 Conclusions

In this intricate analytical framework, meticulous calibration of excess thermodynamic parameters unfolds across the entire compositional spectrum of 2MCH+W, 2MCH+1P, and 2MCH+2P, meticulously undertaken at specific temperature levels. This exhaustive analysis serves as a revelatory exploration, leaving no stone unturned in bringing to light the robust presence of potent hydrogen bonding and dipole-inclusion interactions intricately woven within the fabric of the component molecules. The nuanced revelation of these molecular intricacies sets the stage for a comprehensive understanding of the thermodynamic landscape.

Moreover, the derivation of reduced excess thermodynamic parameters, employing the sophisticated

contemporary RRK polynomial, adds an additional layer of refinement to the investigation. This methodological approach delves deeper into the molecular intricacies, unraveling more specific features. Notably, it sheds light on how the smaller molar masses of water, 1-propanol, and 2-propanol molecules grapple with steric hindrance within the voluminous presence of 2MCH in their respective compositions. The discernment of these interactions becomes more pronounced as the compositions undergo thermal agitations, with reduced excess parameter values exhibiting a discernible downward trend with increasing temperatures.

Within this discerning exploration, the reactivity order of the composites emerges, distinctly articulated as 2MCH(1)+W(2) < 2MCH(1)+1P(2) < 2MCH(1)+2P(2). As a complementary tool in this investigative arsenal, the extraction of partial molar volume from the RRK polynomial provides an additional layer of insight. Within this contextual backdrop, the dynamic interplay of the components is visually represented through 3D graphs, revealing a fascinating narrative. It becomes apparent that intermolecular interactions attain a heightened degree of robustness and intricacy in 2MCH(1)+2P(2) compared to the more subdued dynamics observed in 2MCH(1)+1P(2) & 2MCH(1)+W(2). This exploration transcends the conventional, offering a profound and nuanced understanding of the molecular intricacies at play within these complex compositional systems.

Disclosure Statement

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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