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Thermo-physicochemical investigation of molecular interactions in binary combination (dimethyl carbonate + methyl benzoate)

Measurements and correlation

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Abstract

To probe the nature of interaction and its deeds with temperature in the binary combination (dimethyl carbonate + methyl benzoate), the density (ρ)/speed of sound (u) be established for the total mole fraction array at $T = (308.15, 313.15$ and $318.15)$ K and at atmospheric pressure. Sign with magnitude of evaluated excess molar volume (V_m^E) was inspected and comprehensive analysis elucidated not only pervasiveness of strong molecular interactions between molecules but also its transform with temperature. Additional, strong interactions are properly hold up by partial and excess partial molar volume ($\overline{V}_m$, $\overline{V}_m^E$, $\overline{V}_m^{E,\infty}$). Additionally, relative association ($\boldsymbol{R_A}$), Lennard-Jones repulsive power ($\boldsymbol{n}$), excess isentropic compressibility (κ_s^E), partial and their excess partial molar isentropic compressibility ($\overline{K}_m$, $\overline{K}_m^E$), excess values of isobaric thermal expansion coefficient (α_P^E), isothermal compressibility (k_T^E), intermolecular free length (L_f^E), acoustic impedance (Z^E), ultrasonic speed (u^E) were evaluated and confirmed the deductions of V_m^E. By Redlich–Kister equation, standard deviations are computed through coefficients for excess parameters. At $T = 308.15$ K, V_m^E is correlated by theories of Prigogine–Flory–Patterson (PFP)/topology/Soave–Redlich–Kwong (SRK)/Peng–Robinson (PR) cubic equation of states; prophesied first-order derivatives of thermodynamic potentials; using semi-empirical equations, excess chemical potential/activity coefficients/theoretical speeds are estimated and correlated. Further, microscopic molecular properties are assessed at all temperatures by Sehgal's equations on nonlinear relations.

Keywords Density · Sound speed · Excess parameters · Prigogine–Flory–Patterson theory · Theory of topology · SRK/PR EoS · Activity coefficients · Nonlinear equations

Introduction

The thermo-physicochemical properties of the fluid and their combinations are explored for several reasons, mainly to predict the knowledge pertaining to molecular interactions in liquid amalgamation [1], which comprise enormous employ in theoretical and applied sciences. It is accurately accepted information that the volumetric property is crucial in numerous manufacturing industries in assessments such as in modelling the magnitudes of boilers, condensers and storage deposits etc., [2, 3]. Acoustic examination in liquid blend can be used to ascertain the consequence of arrangement of donor constituents and

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polarity of channel on the constancy of composites which play a noteworthy function in complexation [4] and pattern steady standards of charge transport compounds to compare their stabilities [5]. With the extensive selection of required assets, dual and multicomponent liquid mixtures are of enormous implications in several chemical, manufacturing and biological methods [6]. Further, knowledge of the dependence of volumetric/acoustic speed on the constitution, temperature and pressure is vital in understanding the intermolecular periphery and phase activities of fluids/liquids. Furthermore, several factors are likely to envisage with volumetric/acoustic speed and illustrate its thump which goes from pharmaceuticals to underwater acoustics. Hence, chemicophysical factors play central task in computing nano- to macro-level parameters belonging to binary liquid in study.

The liquid solvents in the contemporary system are elected based on their use in diversified areas. Dimethyl carbonate (DMC) is a eco-friendly liquid; as a consequence, it is recurrently contemplate to be green solvent, used as fuel [7], as a cleaning agent/an electrolyte for high-performance battery expertise [8], it is a strong competitor in fuel engineering due to its lofty oxygen percentage and it has little toxicity, low boiling temperature [9, 10]. Industrially, it is used as a propellant, solvent for sprays, paints and a better lubricant.

Methyl benzoate (carboxylate ester) is a clear colourless liquid that is poorly soluble in water but miscible with organic solvents. Pleasant floral smell which attracts insects and good solvent capability leads to many industrial multifold applications as a perfumery/preservative/pesticide. Additionally, it is widely used in drug tracking: drug sniffing dogs are skilled to reveal the aroma of methyl benzoate which emanate from cocaine hydrochloride in humid atmosphere.

Precise investigations of the physicochemical characteristics of MB with many liquids have been described [11–17]. Sreehari et al. [11] reported density and speed of sound data for (MB + 1-propanol), (MB + 1-butanol/1-pentanol) at $T = (303, 308, 313, 318, 323)$ K. Manapragada et al. [12] reported density, viscosity, and speed of sound data of (methyl benzoate + cyclohexane), (methyl benzoate +*n*-hexane), (methyl benzoate + heptane), and (methyl benzoate + octane at T (303.15, 308.15, and 313.15) K. From this data, excess volume and isentropic compressibility have been estimated. Sreehari et al. [13] reported density, viscosity, and speed of sound values for the binary combination systems of (methyl benzoate + 2-propanol) and (ethyl benzoate + 2-propanol) at temperatures (303.15, 308.15, 313.15, 318.15, and 323.15) K. From these, excess values of isentropic compressibility, molar volume, free length, GiMB's free energy and excess enthalpy have been calculated. Aminabhavi et al. [14] reported densities, refractive indices, speeds of sound, and shear viscosities for (diethylene glycol dimethyl ether + EA/MB/EB + diethyl succinate) are measured at temperatures of (298.15, 303.15, 308.15, 313.15, and 318.15) K. Pandharinath et al. [15] reported densities and viscosities in (*N*,*N*-DMF + toluene/methyl benzoate) at (298.15, 303.15, 308.15, and 313.15) K at atmospheric pressure. Sheu and Tu [16] reported densities, viscosities, refractive indices, and surface tensions for 12 flavour esters including MB were measured from (288.15–358.15) K at atmospheric pressure. Blanco et al. [17] reported densities and viscosities for the two binary combinations of (MB/EB + n-heptane) at different concentrations at (288.15–318.15) K.

Organised explorations of the physicochemical properties of DMC with molecular organic solvents have been reported [18–21]. Lugo et al. [18] accounted the volumetric/ultrasonic speed and assessed isothermal compressibility/isobaric thermal expansion coefficients and internal pressures have been computed using the Tait correlations at (278.15–353.15) K for pressures up to 25 MPa in DMC + octane. Shin et al. [19] assessed the volumetric, optic and kinematic viscosities were measured for (DMC + DPC). Iglesias-Otero et al. [20] reported the optic, volumetric in (DMC + [Bmim][BF4]), while Chen et al. [21] measured volumetric, viscosities and acoustic speed of (γ-GBL + DMC) at (293.15–333.15) K. Excess molar volumes, viscosity deviations, thermal expansion coefficients, bulk Modulus, and the excess Gibbs energy were calculated.

Several applications associated with these solvents and their blend motivated the required extra enormous information on thermodynamic transport characteristics. Literature reviews reveal that no endeavour has been known on (dimethyl carbonate + methyl benzoate). Subsequently, an effort has been demeanour to examine the molecular interactions in (DMC + MB) at $T = (308.15, 313.15$ and $318.15)$ K at atmospheric pressure.

In this expose, besides molecular interaction investigation based on excess properties, an effort has also been made from volumetric, ultrasonic speed of sound rather than calorimetric researches to envisage, for instance: (1) correlation of theoretical $V_{\mathrm{m}}^{\mathrm{E}}$ from Prigogine–Flory–Patterson (PFP), topology; cubic equation of state of Soave–Redlich–Kwong (SRK)/Peng–Robinson (PR) at 308.15 K (2) several excess characteristics (3) first-order derivatives of thermodynamic potentials (4) excess chemical potential by *Margules, Porter, Wilson, Van Laar, NRTL* equations and their correlation at 308.15 K, (5) theoretical speeds using *Nomoto, Vangel, Rao's, Impedence, Jungi* semi-empirical equations and their correlation at 308.15 K. Present investigation also includes an assessment of cohesive energy ΔA, van der Wall's constants (a, b), distance of closest approach (d) from Sehgal's equations

Table 2 Experimental values of density, ρ, ultrasonic speed of sound, u and specific heat (C_p) of pure liquids at atmospheric pressure with the corresponding literature values at $T = (308.15/313.15/318.15)$ K

Liquid	ρ/kg m^{-3}		u/m s^{-1}		C_p/JK^{-1} mol^{-1}
	Expt.	Litt.	Expt.	Litt.	Litt.
Dimethyl carbonate (DMC)					
308.15 K	1050.18	1050.071 [26]	1155.63	1153.7 [28], 1155 [29]	161.30 [31]
313.15 K	1043.50	1043.388 [26]	1134.23	1135.0 [27], 1134 [30]	162.90 [31]
318.15 K	1036.79	1036.687 [26]	1113.09	–	163.00 [31]
Methyl benzoate (MB)					
308.15 K	1070.6	1074.4 [12], 1073.9 [14], 1070.6 [11]	1371.6	1364 [12], 1372 [14], 1371.6 [11]	223.31 [31]
313.15 K	1065.5	1070.3 [12], 1069.0 [14], 1065.5 [11]	1348.4	1348 [12], 1352 [14], 1348.4 [11]	224.30 [31]
318.15 K	1061.2	1061.2 [11]	1326.6	1326.6 [11]	225.28 [31]

impedance (Z^E), isentropic compressibility (κ_s^E), sound speed (u^E), isobaric thermal expansion coefficient (α_P^E), intermolecular free length (L_f^E) are specified in Supplementary file *S*.

Redlich–Kister [35] equation is given by

$$Y_{\text{cal}}^E = x_1(1 - x_1)\sum_{i=1}^{n} A_{i-1}(1 - 2x_1)^{i-1} \tag{5}$$

and is used to obtain coefficients with standard deviations for V_m^E, α_P^E, κ_s^E, k_T^E, L_f^E, Z^E, u^E.

Here, A_{i-1} are called as coefficients obtained by best-fit values of Y_{cal}^E. The standard deviations σ of Y_{cal}^E are given by:

$$\sigma\left(Y_{\text{cal}}^E\right) = \left(\frac{\sum\left(Y_{\text{exp}}^E - Y_{\text{cal}}^E\right)^2}{(m - n)}\right)^{0.5} \tag{6}$$

where m and n are number of investigational data points and coefficients, respectively.

Furthermore, acoustic speeds are computed by semi-empirical relations (given in Supplementary file *S*), namely Nomoto [36], Van Dael [37], Baluja and Parsania [38] and Rao's (specific sound speed) [39].

Results and discussion

Volumetric studies

Experimental densities (ρ)/acoustic speed of sound (u) of binary system dimethyl carbonate (1) + methyl benzoate (2) at different compositions and at $T = (308.15, 313.15$ and $318.15)$ K are depicted in Table 3. It is clear from table that ρ, u values not only raise nonlinearly with the composition of the MB but also their magnitude lessen with rise in temperature. This nonlinear variation of ρ and u with respect to composition of MB and temperature emphatically signifies the divergence from ideal characteristics. This authenticates the prevalence of interactions among (DMC + BB) molecules at $T = (308.15, 313.15$ and $318.15)$ K.

In order to probe the type of interactions present between DMC and MB, excess molar volume V_m^E for various mole fractions of MB at $T = (308.15, 313.15, 318.15)$ K is evaluated from scheduled molar volume (V_m) of Table 3. Scrutiny of Fig. 1 exemplifies that V_m^E has negative values and its magnitude w.r.t temperature follows the trend: $(308.15 < 313.15 < 318.15)$ K. It is a well-known fact that negative V_m^E suggests reduction in volume. For the present circumstances, negative value of V_m^E is overruling with rise in temperatures over total mole fraction of MB for the binary combination (DMC + MB).

A generalised procedure which contributes excess molar volume is laid down and classified as chemical, structural, physical features of the constituent liquids [40–42]. On the basis of this theory, subsequently thorough and yet reasonable qualitative search which suits the present scenario of (DMC + MB) can be discussed.

1. *Chemical* interaction includes dipole–dipole/dipole-induced dipole interaction/hydrogen bonding among the constituents molecules. Presence of these jointly or partly results in negative V_m^E. On the basis of above theory, quest for presence of chemical interaction in (DMC + MB) can be followed as: DMC is a polar solvent comprising a dipole moment $\mu = 0.90$ D and methyl benzoate is relatively high polar molecule with dipole moment $\mu = 1.92$ D. Since the magnitude of interaction among the constituents also depends on the values of μ of the interacting molecules [43], hence high dipole moment associated with the MB molecule may attract DMC, causing Keesom-type interactions

pertinent to *Hartmann–Balizar* and *Ballou* nonlinearity parameters at (308.15, 313.15, 318.15) K.

Experimental

Chemicals

Dimethyl carbonate and methyl benzoate (A.R. grade) were attained from Sigma-Aldrich (India) and Merck Co. (Germany), respectively. The liquids were decontaminated as expressed in the literature [22–24]. Preceding to experiment, the samples were desiccated for no less than 72 h under 0.1 Pa pressure and optimal temperature (opening at 300.15 K and afterwards elevated in bit by bit over a 6 h duration to 320 K). The H_2O in DMC, MB was probed by Karl Fisher titrator (Mtrohm, 890 Titrando) [25]. Also, the binary mixtures are purified by distillation. The H_2O estimation of each section is ascertained and established to be in the limit of < 150 ppm. The liquids after final purification were > 99% pure. This is not only established by the GLC but also confirmed with volumetric and acoustic speed data available in the literature [11, 12, 14, 26–30] at $T = (308.15/313.15/318.15)$ K. Specific heat for both the liquids is taken from the literature [31]. In the end, the pure liquids were stock up over activated 0.4 nm molecular sieves and in dark bottles. The suppliers and purity of liquids are given in Table 1. The comparison is precised in Table 2 and accord among the investigational and the literatures were established to be proper.

Apparatus and procedure

The weighing has been made by means of a METTLER TOLEDO (Switzerland make) AMB5-S/FACT digital balance with an accuracy of ± 0.01 mg. The uncertainty in the mole fraction is 10^{-4}. Densities (ρ) have been measured by 10 cm^3 two stem double-walled Parker & Parker type pycnometer [32]. The modus operandi for measuring ρ has been explained in our previous papers [33, 34]. The temperature was kept constant by means of circulating water around the liquid cell of a Mittal type thermostat controlled to ± 0.01 K.

Theory

Experimental ρ and u of (DMC + MB) system for entire miscibility w.r.t $T = (308.15, 313.15$ and $318.15)$ K under 101.3 kPa pressure are specified in Table 3. Excess parameters are evaluated from ρ and u data through thermodynamic relations specified below.

The excess molar volume is specified by

$$V_{\mathrm{m}}^{\mathrm{E}} = \left[\frac{\sum_{\mathrm{i}=1}^{2}(x_{\mathrm{i}}M_{\mathrm{i}})}{\rho}\right] - \left[\frac{x_1 M_1}{\rho_1}\right] - \left[\frac{x_2 M_2}{\rho_2}\right] \tag{1}$$

where M_1 and M_2 are the molecular weights, x_1 and x_2 are the mole fractions of MB and DMC, respectively; ρ_1, ρ_2 and ρ are the densities of MB, DMC and the combination, respectively.

The Lennard-Jones potential is specified by:

$$\emptyset(r) = \left[\frac{-A}{r^6} + \frac{B}{r^{\mathbf{n}}}\right]$$

Here, $\boldsymbol{n}$ describes the magnitude of repulsive force among binaries and is called as L-J repulsive power term (n) specified by

$$n = \left(\frac{6 * V_{\mathrm{m}}}{V_{\mathrm{a}}}\right) - 13 \tag{2}$$

where V_{m} and V_{a} are molar and available volumes, respectively.

Available volume (V_{a}) is specified by

$$V_{\mathrm{a}} = V_{\mathrm{m}}\left(1 - \frac{u}{u_{\infty}}\right) \tag{3}$$

where $u_{\alpha} = 1600$ m s^{-1}.

Relative association (R_{A}) is specified by

$$R_{\mathrm{A}} = \frac{\rho_{\mathrm{s}}}{\rho_{\mathrm{o}}} * \left(\frac{u_{\mathrm{o}}}{u}\right)^{1/3} \tag{4}$$

where ρ_{o} and ρ_{s} are density of methyl benzoate and combination, respectively.

Expressions for partial molar volumes ($\overline{V}_{\mathrm{m},1}$, $\overline{V}_{\mathrm{m},2}$), excess partial molar volumes ($\overline{V}_{\mathrm{m},1}^{\mathrm{E}}$, $\overline{V}_{\mathrm{m},2}^{\mathrm{E}}$), partial molar volumes at infinite dilution ($\overline{V}_{\mathrm{m},1}^{\infty}$, $\overline{V}_{\mathrm{m},2}^{\infty}$), excess partial molar volumes at infinite dilution ($\overline{V}_{\mathrm{m},1}^{\mathrm{E},\infty}$, $\overline{V}_{\mathrm{m},2}^{\mathrm{E},\infty}$) [33] and relevant equations pertinent to excess values of acoustic

Table 1 List of chemicals with details of provenance, CAS number and mass fraction purity

Chemical	Provenance	CAS number	Purification method	Mass fraction purity	Analysis method
Dimethyl carbonate	Sigma-Aldrich, India	61638-6	Distillation	0.99	Gas liquid chromatography
Methyl benzoate	Merck Co. Inc, Germany	93-58-3	Distillation	0.99	Gas liquid chromatography

Table 3 Experimental density (ρ)/speed of sound (u) and computed Lennard-Jones repulsive exponent (n)/relative association (R_A)/molar volume (V_m) and excess values of isobaric thermal expansion coefficient (α_p^E)/free length (L_f^E)/isentropic compressibility (κ_s^E) with mole fraction (x_1) of MB in the binary liquid mixture of {DMC + MB} from T = (308.15/313.15/318.15) K at pressure P = 101.3 kPa

x_1	ρ/kg m^{-3}	u/m s^{-1}	n	R_A	$V_m/10^{-6}$ m^3 mol^{-1}	$\alpha_p^E/10^{-3}$ K^{-1}	$L_f^E/10^{-10}$ m	$\kappa_s^E/10^{-10}$ Pa^{-1}
T = 308.15 K								
0.0000	1050.18	1155.63	8.6036	1.0000	85.7758	0.0000	0.0000	0.0000
0.1137	1053.94	1192.63	10.5661	1.0142	90.4400	− 0.0271	− 0.1203	− 0.0049
0.2134	1056.93	1222.46	12.4274	1.0255	94.5298	− 0.0451	− 0.1886	− 0.0078
0.3343	1060.18	1255.32	14.8522	1.0378	99.4939	− 0.0596	− 0.2337	− 0.0099
0.4321	1062.50	1279.27	16.9316	1.0466	103.5170	− 0.0657	− 0.2452	− 0.0106
0.5023	1064.00	1295.00	18.4755	1.0524	106.4107	− 0.0666	− 0.2417	− 0.0106
0.6111	1066.05	1316.98	20.9197	1.0603	110.9084	− 0.0631	− 0.2191	− 0.0098
0.7432	1068.08	1339.73	23.8850	1.0684	116.3955	− 0.0505	− 0.1671	− 0.0076
0.8331	1069.17	1352.75	25.8273	1.0730	120.1498	− 0.0368	− 0.1179	− 0.0054
0.9112	1069.94	1362.44	27.4112	1.0763	123.4266	− 0.0213	− 0.0669	− 0.0031
1.0000	1070.60	1371.63	29.0370	1.0794	127.1717	0.0000	0.0000	0.0000
T = 313.15 K								
0.0000	1043.50	1134.23	7.6110	1.0000	86.3249	0.0000	0.0000	0.0000
0.1137	1047.79	1171.15	9.3855	1.0149	90.9703	− 0.1139	− 0.1512	− 0.0060
0.2134	1051.18	1200.87	11.0525	1.0267	95.0467	− 0.1890	− 0.2362	− 0.0096
0.3343	1054.81	1233.59	13.2000	1.0395	99.9998	− 0.2496	− 0.2914	− 0.0122
0.4321	1057.37	1257.39	15.0199	1.0487	104.0191	− 0.2745	− 0.3047	− 0.0130
0.5023	1059.00	1273.00	16.3575	1.0547	106.9133	− 0.2791	− 0.2995	− 0.0129
0.6111	1061.17	1294.76	18.4510	1.0628	111.4177	− 0.2646	− 0.2703	− 0.0119
0.7432	1063.25	1317.22	20.9490	1.0710	116.9243	− 0.2119	− 0.2052	− 0.0092
0.8331	1064.30	1330.02	22.5580	1.0755	120.6997	− 0.1542	− 0.1444	− 0.0066
0.9112	1064.99	1339.50	23.8521	1.0788	124.0007	− 0.0895	− 0.0818	− 0.0038
1.0000	1065.50	1348.40	25.1558	1.0817	127.7804	0.0000	0.0000	0.0000
T = 318.15 K								
0.0000	1036.79	1113.09	6.7162	1.0000	86.8836	0.0000	0.0000	0.0000
0.1137	1042.16	1149.72	8.3201	1.0161	91.4617	− 0.2022	− 0.1986	− 0.0078
0.2134	1046.33	1179.23	9.8153	1.0288	95.4876	− 0.3353	− 0.3089	− 0.0124
0.3343	1050.69	1211.75	11.7261	1.0425	100.3923	− 0.4423	− 0.3792	− 0.0157
0.4321	1053.67	1235.43	13.3323	1.0522	104.3849	− 0.4858	− 0.3948	− 0.0166
0.5023	1055.50	1250.98	14.5056	1.0585	107.2678	− 0.4942	− 0.3868	− 0.0165
0.6111	1057.84	1272.70	16.3306	1.0669	111.7691	− 0.4683	− 0.3474	− 0.0151
0.7432	1059.85	1295.16	18.4921	1.0752	117.2985	− 0.3750	− 0.2620	− 0.0116
0.8331	1060.71	1308.00	19.8771	1.0796	121.1082	− 0.2727	− 0.1835	− 0.0083
0.9112	1061.12	1317.55	20.9885	1.0826	124.4525	− 0.1585	− 0.1035	− 0.0047
1.0000	1061.20	1326.59	22.1121	1.0852	128.2982	0.0000	0.0000	0.0000

(attractive interactions among dipoles). Additionally, establishment of H-bond is not possible though DMC possess hetero atom O (–C=O) but MB lack hydroxyl groups. In the contemporary exploration, likelihood of Keesom-type forces which happen due to dipole moment of constituents deliberate strong interactions giving rise to negative V_m^E [44]. Hence dipole–dipole interactions are surely existing among (DMC + MB).

2. The *structural* participation happened due to dissimilarity in molar and free volumes of the constituents; this permits the interstitial accommodation and geometrical fitting of smaller constituent into the bigger, producing negative V_m^E values. As regards the structural effect, V_m of pure constituents DMC and MB are 85.7758 ($\times$ 10^{-6} m^3 mol^{-1}) and 127.1717 ($\times$ 10^{-6} m^3 mol^{-1}) at 308.15 K, respectively, which

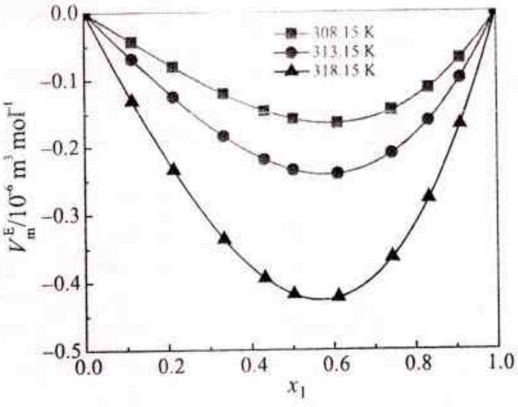

Fig. 1 Plots of excess molar volume (V_m^E) against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

may permit the constituent molecules to fit into each others arrangements make sinking of V_m value of the combination. The same tendency also holds good at (313.15, 318.15) K. This type of trend was also postulated by the other researchers to interpret negative V_m^E [45, 46].

3. The *physical* contributions possess dispersion forces which consist of breaking of the structure of one or both of the constituents in the solution/loss of dipolar alliance among the constituents of liquids/steric hindrance of the molecules and H-bond rupture. Presence of these jointly or partly leads to positive V_m^E [47, 48]. For the present (DMC + MB) system, the resultant V_m^E is negative indicating that physical contribution between molecules is not much influential though weak van der Wall's dispersion forces are readily available.

From Fig. 1, it is observed that at ~ 0.5 mol fraction of MB, magnitude of V_m^E rises as the temperature hikes from (308.15 to 318.15) K. The observed drift in V_m^E shows that with rise in temperature, strength of interaction among the liquid constituents also rises. This is due to the fact that thermal energy is proportional to temperature. Hence, as temperature rises, consequently thermal energy of molecules also rises. This increase in thermal energy stimulates the constituents which causes the union of dissimilar components [49, 50]. This explains observed strength of interactions with temperature to track: (318.15 > 313.15 > 308.15) K. In short, sign and magnitude of V_m^E with mole fraction / temperatures are the result of collective consequence of above suggested aspects of dipole–dipole interactions, interstitial accommodation of DMC molecules into the voids of MB molecules. These together lead to the observed strong interactions to track the trend: (318.15 > 313.15 > 308.15) K.

An additional and yet crucial thermodynamic extent that specifies how an extensive assets of a mix vary with changes in the molar composition of the combination at stable pressure/temperature can be inspected through partial molar volume. It not only equips critical knowledge concerning the solute–solvent interactions but also the solute arrangement in mixture. The existing strong interactions in (DMC + MB) are appropriately simulated in their partial molar volume analysis. $\overline{V}_{m,1}$ and $\overline{V}_{m,2}$ of Table 4 for the constituents in the combination are smaller than their pure status; this stipulates contraction of volume of solvent molecules in the amalgamation procedure of MB and DMC constituents. Figure 2 stands for the excess partial molar volumes for DMC ($\overline{V}^E_{m,2}$) and MB ($\overline{V}^E_{m,1}$) in the amalgamation with x_1 of MB at $T = (308.15, 313.15, 318.15)$ K. Inspection of Fig. 2 illustrates that $\overline{V}^E_{m,1}$ and $\overline{V}^E_{m,2}$ values are negative for the entire temperatures which also hints that interaction is stronger among MB and DMC molecules. Table 5 depicts that $\overline{V}^{E,\infty}_{m,1}$ and $\overline{V}^{E,\infty}_{m,2}$ are negative and thus support the inferences haggard from the excess molar volume. Thus, lesser $\overline{V}_{m,1}$ (MB), $\overline{V}_{m,2}$ (DMC) and negative ($\overline{V}^E_{m,1}$, $\overline{V}^E_{m,2}$, $\overline{V}^{E,\infty}_{m,1}$ and $\overline{V}^{E,\infty}_{m,2}$) authenticate the existence of strong interactions between (DMC + MB) system. In addition, as temperature rises from (308.15 to 318.15) K, the magnitude of $\overline{V}_{m,1}$(Table 4)/$\overline{V}^{\infty}_{m,1}$ and $\overline{V}^{E,\infty}_{m,1}$ (Table 5) of the component (MB) also rises. This tendency bears a resemblance to the trend of V_m^E w.r.t to temperature and thus supports the formerly deduction of rise in strong interaction with temperature as: (318.15 > 313.15 > 308.15) K.

Theoretical analysis of V_m^E

An endeavour has been prepared to assess theoretical V_m^E from statistical theory of Prigogine–Flory–Patterson (PFP), graph theory of topology and Soave–Redlich–Kwong (SRK)/Peng–Robinson (PR) cubic equation of state at $T = 308.15$ K in the binary combination (DMC + MB). The calculated theoretical values are finally correlated with experimental V_m^E values at 308.15 K.

V_m^E through Prigogine–Flory–Patterson (PFP) theory

V_m^E computed from Prigogine–Flory–Patterson (PFP) theory has three parts namely the free volume, the characteristic pressure, the energy of interaction namely $V_m^E(\mathrm{fv})$, $V_m^E(\mathrm{ip})$, $V_m^E(\mathrm{int})$ respectively. All equations pertinent to these terms are specified in the literature [51–54]. The contact interaction term labelled as the Flory parameter χ_{12}

Table 4 Partial molar volumes $\overline{V}_{m,1}$ (MB) and $\overline{V}_{m,2}$ (DMC) against mole fraction (x_1) of MB for binary mixture (dimethyl carbonate (2) + methyl benzoate (2)) at T = (308.15/313.15/318.15) K

x_1	$\overline{V}_{m,2}$ /10^{-6} m^3 mol^{-1}	$\overline{V}_{m,1}$	$\overline{V}_{m,2}$	$\overline{V}_{m,1}$	$\overline{V}_{m,2}$	$\overline{V}_{m,1}$
	T = 308.15 K		T = 313.15 K		T = 318.15 K	
0.0000	85.7758	126.2920	86.3249	126.3103	86.8836	126.4276
0.1137	85.7665	126.5525	86.3026	126.6983	86.8445	126.7776
0.2134	85.7287	126.7561	86.2503	127.7686	86.7579	127.8221
0.3343	85.6555	126.9364	86.1577	127.4148	86.6055	127.6311
0.4321	85.5923	127.0324	86.0696	127.5569	86.4559	127.8737
0.5023	85.5496	127.0807	86.0039	127.6321	86.3404	128.0058
0.6111	85.4836	127.1323	85.9042	127.7120	86.1593	128.1514
0.7432	85.3884	127.1678 .	85.7979	127.7628	85.9579	128.2505
0.8331	85.3189	127.1767	85.7437	127.7767	85.8451	128.2824
0.9112	85.2870	127.1756	85.7165	127.7803	85.7670	128.2947
1.0000	85.3647	127.1717	85.7208	127.7804	85.6979	128.2982

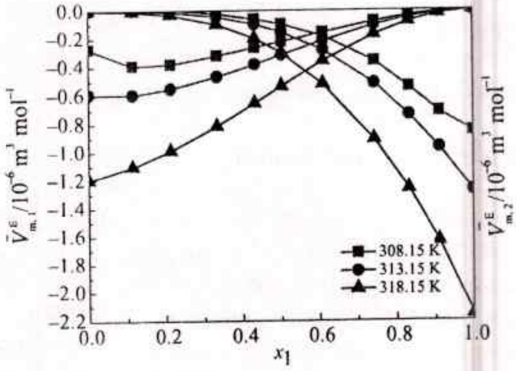

Fig. 2 Plots of excess partial molar volumes $\overline{V}^{E}_{m,1}$ (MB) and $\overline{V}^{E}_{m,2}$ (DMC) against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

Table 5 Partial molar volumes ($\overline{V}^{\infty}_{m,1}$, $\overline{V}^{\infty}_{m,2}$) and excess partial molar volumes ($\overline{V}^{E,\infty}_{m,1}$, $\overline{V}^{E,\infty}_{m,2}$) of the components at infinite dilution for binary mixture (dimethyl carbonate (2) + ethyl benzoate (2)) at T = (308.15/313.15/318.15) K

T/K	$\overline{V}^{\infty}_{m,2}$ /10^{-6} m^3 mol^{-1}	$\overline{V}^{\infty}_{m,1}$	$\overline{V}^{E,\infty}_{m,2}$	$\overline{V}^{E,\infty}_{m,1}$
308.15	85.5007	126.2920	− 0.8797	− 0.2750
313.15	85.5326	126.4103	− 1.2701	− 0.5922
318.15	85.6868	126.5276	− 2.1706	− 1.1968

was assessed from experimental V^{E}_{m} and found to be negative. This negative χ_{12} advocates that the arising interactions in (DMC + MB) are strong. Table 6 includes factors of the pure constituents used in PFP theory estimation. Table 7 reports the interaction parameter χ_{12} and the calculated values of interaction at equimolar concentration. It is clear from the table that the V^{E}_{m}(ip) term which signifies the characteristic pressure is negative for (DMC + MB) and is leading because of its higher magnitude in comparison with other two contributions. Thus characteristic pressure play a key factor for the sign and magnitude of the excess molar volume computed through PFP theory for (DMC + MB) system at 308.15 K.

V^{E}_{m} through theory of topology

According to mathematics, topological indices are authoritative tools to envisage organic compounds in biological manners, pharmacological and toxicological properties. Theory of chemical topology gives the entirety of information enclosed in the constituents [55, 56], and its complete concept is obtainable in references [57–60]. Since V^{E}_{m} reflects the packing of the constituent molecules, hence topology can be applied to predict extract information about V^{E}_{m}. For the present situation, topology theory has been applied to estimate V^{E}_{m} in (DMC + MB) system at 308.15 K. The equations pertinent to this theory are mentioned in Supplementary file ***S***. The parameters α_{12}, $\left({}^{3}\xi_{i}\right)$ or $\left({}^{3}\xi_{i}\right)_{m}$ (l = 1 or 2) present in this theory are recorded **in** Table 8.

Table 6 Characteristic and reduced parameters for the pure components at T = (308.15/313.15/318.15) K used in PFP theory

Component	T/K	$\tilde{V}$	P^*/ 10^6 J mol^{-1}	V^*/ 10^{-6} m^3 mol^{-1}
DMC	308.15	1.3083	685.7276	65.56089
MB	308.15	1.2603	737.6278	100.9086

Table 7 PFP interaction parameter, χ_{12}, and calculated values of the three contributions from the PFP theory with experimental excess molar volumes at equimolar composition for (DMC + MB) system at T = (308.15/313.15/318.15) K

T/K	$\chi_{12}/10^6$ J m^{-3}	V_m^E(int) /10^{-6} m^3 mol^{-1}	V_m^E(fv)	V_m^E(ip)
308.15	− 1.52828	− 0.02183	− 0.06697	− 0.06912

V_m^E through Soave–Redlich–Kwong (SRK) and Peng–Robinson (PR) cubic equation of state

Soave–Redlich–Kwong (SRK)/Peng–Robinson (PR) cubic equation of state are combined and specified as

$$P = \frac{RT}{V_m - b} - \frac{a(T)}{(V_m + \delta_1 b)(V_m + \delta_2 b)} \tag{7}$$

where $a(T)$ and b are the attractive and repulsive terms, respectively, V_m is the molar volume, P represents the pressure of the system, and δ_1, δ_2 are two parameters and its values for both the models are

$$\text{For SRK, } \begin{cases} \delta_1 = 1 \\ \delta_2 = 0 \end{cases} \text{ and}$$

$$\text{For PR, } \begin{cases} \delta_1 = 1 + 2 \\ \delta_2 = 1 - 2 \end{cases}$$

The wide-ranging knowledge for computation of factors present in SRK and PR is mentioned by Soave [61] and Peng and Robinson [62], respectively.

Mixing rules applied are

$$\begin{matrix} a \\ b \end{matrix} = \begin{cases} \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j \left(1 - k_{ij}\right)\left(a_i a_j\right)^{0.5} \\ x_i b_i + x_j b_j \end{cases}$$

where x_i's are compositions of constituents, and k_{ij} is the adjustable interaction parameter. Here, the computed values through EoS firmly authenticate on the interaction k_{ij}/critical parameters [63, 64] (listed in Table 9). In the present study, density is estimated by SRK/PR equations and therefore molar volume, excess molar volume are evaluated from Eq. (1). Furthermore, we have taken $k_{ij} = -0.0075/-0.0100$ for SRK/PR, respectively. The key in choosing k_{ij} value is based on new approach of equalising calculated and experimental excess molar volume at equimolar mole fraction, i.e. $x_1 = 0.5000$ at 308.15 K.

Figure 3 shows the comparison among experimental and theoretical V_m^E evaluated from theories of Prigogine–Flory–Patterson (PFP) (standard deviation: 0.0045)/topology (standard deviation: 0.0043), cubic equation of states of Soave–Redlich–Kwong (SRK) (standard deviation: 0.0047)/Peng–Robinson (PR) (standard deviation: 0.0048) at 308.15 K. When compared to experimental V_m^E, theoretically evaluated values correctly predicted the sign but with different magnitudes of excess molar volumes. It is clear from Fig. 3 and values of standard deviation that the SRK, PR equations give almost similar result in the assessment of excess molar volume for (DMC + MB) but with different k_{ij} values. Additionally, we construe that small standard deviation in V_m^E is evaluated by theory of topology contrast sensibly with experimental V_m^E and thus can be exploit to get details of existing molecular interactions between mixed states of ethers.

Thermo-acoustic studies

Relative association ($\boldsymbol{R}_\mathbf{A}$) assigns an outline concerning the possibility of association of constituents. Its change with composition provides a sketch related to molecular interaction between hetero molecules. The rise in $\boldsymbol{R}_\mathbf{A}$ with composition specifies (1) divide of the coupled solvent constituent due to mixing of solute and (2) the salvation of solute molecule. Thus, from Table 3, rise in $\boldsymbol{R}_\mathbf{A}$ with rise in x_1(MB) shows the occurrence of strong interaction among (DMC + MB) at all temperatures. Lennard-Jones repulsive exponent ($\boldsymbol{n}$) decreases with decrease of x_1 (MB) and rise in temperature. Since $\boldsymbol{n}$ depicts the extent of repulsive force between liquid molecules, its decrease with x_1 and temperature explains the superiority of attraction over repulsion in (DMC + MB) at all temperatures. Thus, for the present system, both $\boldsymbol{R}_\mathbf{A}$ and $\boldsymbol{n}$ not only supports the supremacy of attractive strong forces between (DMC + MB) but also their strength track: (318.15 > 313.15 > 308.15) K.

The study also covers an investigation on the understanding of dependence of x_1 (MB) and temperature on isentropic

Table 8 Values α_{12} and $(3_{\xi_1})\left[= (3_{\xi_1})_m\right]$, $(3_{\xi_2})\left[(3_{\xi_2})_m\right]$ pertinent to Graph theory for (DMC + MB) mixture at T = 308.15 K

Liquid	P_C	T_C/K	ω
DMC [63]	49.1	557	0.346
MB [64]	40.2	702	0.4048

Table 9 Values of critical parameters of pressure (P_C)/temperature (T_C) and acentric factors (ω) for DMC and MB at 308.15 K

T/K	α_{12} /10^{-6} m^3 mol^{-1}	3_{ξ_1}	3_{ξ_2}
308.15	1.3411	1.0007	1.0013

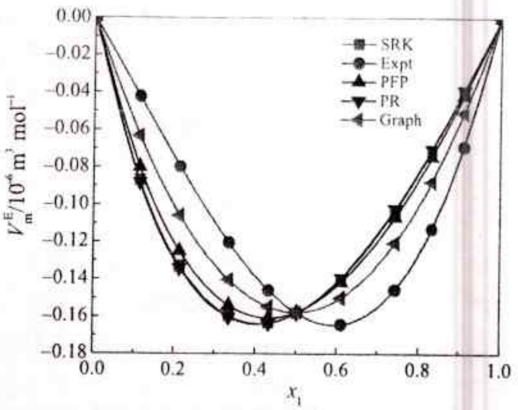

Fig. 3 V_m^E evaluated by experimental and different theories against mole fraction (x_1) of MB in the mixture with DMC at $T = 308.15$ K

compressibility (κ_S)/excess isentropic compressibility (κ_s^E). It is obvious from Table 3 that κ_s^E have negative sign over the whole x_1 of MB and magnitude of κ_s^E increases with rise in temperature. According to Fort and Moore [65], negative κ_s^E direct that the blend is in compressed state, i.e. constituents in the blend are more effectively packed than in their pure form. This is possible only if DMC occupies the space of voids created by MB. Consequently, this paves the way to the molecular coalition and causes the compact structure in binary combinations. This compressed arrangement clearly stresses the existence of strong interactions between (DMC + MB). Thus, the conclusion of κ_s^E also supports the occurrence of strong specific interaction in the combination and the negative κ_s^E increases with temperature track the order: (318.15 > 313.15 > 308.15) K. This advocates the increase in strong interactions with rise in thermal energy of molecules [66].

The explored values K_S, $\overline{K}_{m,1}$, $\overline{K}_{m,2}$, $\overline{K}_{m,1}^E$, $\overline{K}_{m,2}^E$ are presented in Supplementary Table S1. At this stage, $K_s (= \kappa_S V_m)$, $\overline{K}_{m,1}$, $\overline{K}_{m,2}$ and $\overline{K}_{m,1}^E$, $\overline{K}_{m,2}^E$ are called as molar, partial molar and excess partial molar isentropic compressibilities, respectively. From this table, $\overline{K}_{m,1}$ (MB) and $\overline{K}_{m,2}$(DMC) for both the constituents in the combination are lesser than their individual K_s values. This reconfirms condensed arrangement (reduction in volume) in the mixture [67] and is probable only if strong interactions be present between DMC and MB. Additionally, examination of Table S1 illustrates that magnitude of negative excess partial molar isentropic compressibilities rises w.r.t temperature and this behaviour is in full accord with variant of κ_s^E with temperature in the system.

It is evident from Table 3, Fig. 4 that variation of negative excess isobaric thermal expansion coefficient (α_P^E), negative intermolecular free length (L_f^E), positive acoustic impedance (Z^E) with composition and temperature also emphasises the conclusions of dominance of strong interactions and rise in their strength with temperature.

The change of excess speed of sound (u^E) with x_1 of MB at $T = (308.15/313.15/318.15)$ K is drawn as Fig. 5. It is well-known fact that strong interactions existing between hetero molecules of a binary liquid mixture causes structure making effect which leads to closely packed arrangement [68]. Sound waves need medium (material particles) to propagate consequently its speed rises as compact arrangement between binary liquids is dominant. For such circumstances of closely packed structure, magnitude of excess ultrasonic speed will become positive [69]. If the same theory is applied to the present system, observed positive u^E emphasises the status of closely packed arrangement between DMC and MB. Thus, u^E supports the existence of strong interaction between molecules in study. Moreover, as temperature rises from 308.15 to 318.15 K, magnitude of u^E also rises; subsequently, possibility of shrinkage of resultant arrangement is more favourable. Thus, the strength of strong interactions rises with rise in temperature which supports the observed trend of strong interactions: (318.15 > 313.15 > 308.15) K. The sign and changes with temperature pertinent to u^E are conflicting to that established by κ_s^E, and these are caused by identical reasons as was conferred for κ_s^E.

From Fig. 6, excess isothermal compressibility (k_T^E) illustrate analogous fashion similar to κ_s^E at $T = (308.15/313.15/318.15)$ K. Negative sign and magnitude of k_T^E are accredited to the compressibility of molecules in the mix. This nearer movement of distinct constituents [70] in the (DMC + MB) system reproduces the presence of strong interaction at (308.15/313.15/318.15) K.

The excess properties V_m^E, α_P^E, κ_s^E, k_T^E, L_f^E, Z^E, u^E are used in Redlich–Kister equation, and standard deviation is estimated through coefficients (Table 10) for the binary system (DMC + MB) at $T = (308.15/313.15/318.15)$ K.

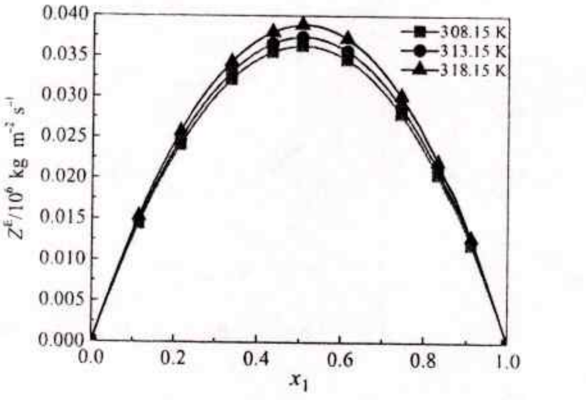

Fig. 4 Plots of excess acoustic impedance (Z^E) against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

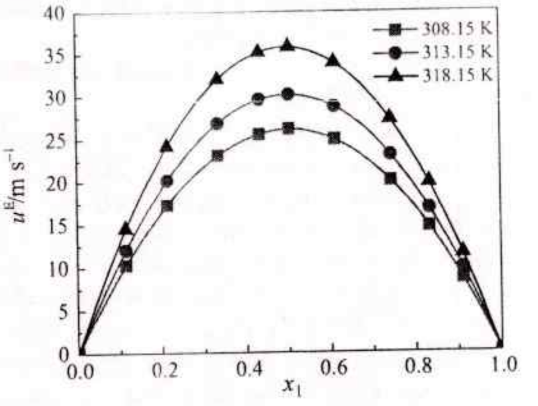

Fig. 5 Plots of excess ultrasonic speed of sounds (u^E) against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

Derivatives of thermodynamic potentials

Fundamental functions in thermodynamics are called as thermodynamic potentials. These potentials are functions of eigenvariables, and by differentiation, we can obtain vital information which describes the system. This derived information relates the physicochemical properties of systems with thermodynamic potentials and can be utilised not only to analyse the progress of thermodynamic processes but also to predict their variation with pressure and temperature. Usually, thermodynamic potentials are measured by calorimeters. They give error in measurement due to loss of heat energy to surroundings. However, the advantage of information of chemicophysical characteristics above calorimetric testing has significance in all the branches of science, and its conclusions are frequently useful in several chemical, pharmaceutical and manufacturing methods [6]. Because of these applications in miscellaneous sections, certain thermodynamic potential derivatives [71] for (DMC + MB) are computed by density/speed of sound and are shown in Table 11. Implication of thermodynamic derivatives can be understood from Figs. 7, 8 for $\left(\frac{\partial V_m^E}{\partial T}\right)_P$, $\left(\frac{\partial H_m^E}{\partial P}\right)_T$, respectively, plotted against x_1 of MB at (308.15/313.15/318.15) K. It is to be noted that $\left(\frac{\partial V_m^E}{\partial T}\right)_P$ and $\left(\frac{\partial H_m^E}{\partial P}\right)_T$ are analogous with the composition and temperature but accompanied by conflicting sign. Negative values of $\left(\frac{\partial V_m^E}{\partial T}\right)_P$ for the combination are certainly owing to strong interactions acting among (DMC + MB) of the combination as was explained at V_m^E. The positive values obtained for the variation of excess molar enthalpy with pressure at constant temperature $\left(\frac{\partial H_m^E}{\partial P}\right)_T$ in the complete mole fraction reveals raise of attraction forces among two constituents with rise in pressure. Hence, reduction in V_m of the combination is highly probable because of rising pressure. Further, from Table 11, values of $\left(\frac{\partial S_m^E}{\partial P}\right)_T$ are negative and its negative magnitude increases with the increase in pressure at constant temperature. This trend indicates that disorder in arrangement of DMC + MB decreases with the increase in pressure as entropy is a measure of disorder in arrangement. This indicates the fact that fitting in voids is more favourable causing the system to be more ordered and is possible only if the interaction between molecules is strong. Thus, $\left(\frac{\partial S_m^E}{\partial P}\right)_T$ trend also supports the conclusions drawn by excess parameters pertinent to nature of interactions.

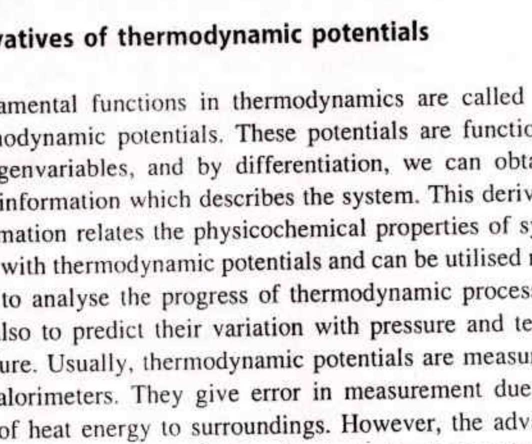

Fig. 6 Plots of excess isothermal compressibility (k_T^E) against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

Excess chemical potential (μ^E)

Excess chemical potential is the vital thermodynamic parameter for phase equilibrium estimations and is useful for chemical separation process. In a chemical reaction/phase transition, it specifies absorption/release of energy. By means of thermodynamic models, the imperfectness (arises due to molecular interactions and forces performing between different molecules in the binary solution) of the liquid phase in liquid part is generally expressed by liquid-excess chemical potential and is accounted by liquid-phase excess chemical potential. This made to evaluate μ^E using *Margules* (standard deviation: 0.0006), *Porter* (standard deviation: 0.0091), *Wilson* (standard deviation: 0.0084), *Van Laar* (standard deviation: 0.0027), *NRTL* (standard deviation: 0.0007) [6, 72] and are plotted in Fig. 9 at $T = 308.15$ K. μ^E computed through Margules equation has small standard deviation when compared to other models.

Table 10 Redlich–Kister coefficients of excess properties and corresponding standard deviations for the binary system (dimethyl carbonate (2) + methyl benzoate (1)) at different temperatures

Property	T/K	A_0	A_1	A_2	A_3	A_4	$\sigma(Y^E)$
$V_m^E/10^{-6}$ m^3 mol^{-1}	308.15	− 0.6302	− 0.2607	− 0.0333	− 0.0416	0.0861	0.0002
	313.15	− 0.9384	− 0.3367	− 0.0010	− 0.0023	0.0083	0.0002
	318.15	− 1.6708	− 0.4860	− 0.0021	− 0.0009	− 0.0108	0.0002
$\kappa_s^E/10^{-10}$ Pa^{-1}	308.15	− 0.9677	0.2254	− 0.0822	0.0112	0.0114	0.0002
	313.15	− 1.1986	0.2996	− 0.0916	0.0189	− 0.0142	0.0003
	318.15	− 1.5490	0.4191	− 0.1333	0.0381	− 0.0103	0.0004
$k_T^E/10^{-10}$ pa^{-1}	308.15	− 2.7613	− 0.4412	− 0.1186	− 0.0128	− 0.0145	0.0004
	313.15	− 5.6795	− 1.0849	− 0.5971	0.0239	− 0.0350	0.0015
	318.15	− 7.7976	− 2.2698	− 1.7681	0.0158	− 0.0948	0.0040
u^E/m s^{-1}	308.15	104.32	− 1.81	0.40	− 1.04	− 1.26	0.02
	313.15	120.56	− 0.49	0.70	− 0.29	− 1.08	0.03
	318.15	143.16	1.78	0.35	− 0.33	0.47	0.02
L_f^E /10^{-11} m	308.15	− 0.0424	− 0.0059	− 0.0014	− 0.00047	− 0.00055	0.00001
	313.15	− 0.0517	− 0.0083	− 0.0030	− 0.00011	0.00077	0.00001
	318.15	− 0.0660	− 0.0122	− 0.0029	0.00013	− 0.00053	0.00002
$Z^E/10^6$ kg m^{-2} s^{-1}	308.15	0.1450	− 0.0028	− 0.0004	0.0001	0.0001	0.0001
	313.15	0.1495	− 0.0033	− 0.0006	− 0.0002	0.0003	0.0001
$\left(\frac{\partial V_m^E}{\partial T}\right)_P$ /10^{-9} m^3 mol^{-1} K^{-1}	308.15	− 19.2385	− 7.85609	9.642993	11.6637	− 21.2368	0.0029
	313.15	− 104.099	− 22.5913	4.221182	4.1748	− 11.2291	0.0168
	318.15	− 188.95	− 37.1459	− 4.12043	− 3.4701	3.3718	0.0338
$\left(\frac{\partial H_m^E}{\partial P}\right)_T$ /10^{-6} J mol^{-1} Pa^{-1}	308.15	5.28302	2.691055	− 2.95663	− 3.5983	6.5530	0.0014
	313.15	31.6514	7.379576	− 1.00539	− 1.2129	3.1874	0.0034
	318.15	58.42918	12.56363	0.472624	0.7334	0.5237	0.0314

Activity coefficients (γ)

The activity coefficient has extensive relevance in industrial design purposes like typify the performance of liquid blends, assessment of reciprocal miscibility, provide information for the quantitative thermodynamicist, diagnostic chromatographers, choosing an economical extraction process and extractive distillation developments, consistent fabrication of distillation and separation methodology, and computation of Henry constants/partition coefficients. Investigational statistics are often rare over the choice of specifications of pursuit; so, the requisite statistics have to be approximate via diversity of methods. This prepared us to endeavour estimate of activity coefficients of (DMC + MB) at 308.15 K. For the present system, activity coefficients are evaluated by *Margules* (standard deviation: 0.0005), *Porter* (standard deviation: 0.0090), *Wilson* (standard deviation: 0.0082), *Van Laar* (standard deviation: 0.0025), *NRTL* (standard deviation: 0.0006) equations are plotted in Fig. 10. Activity coefficients computed through Margules equation has small standard deviation when compared to other models.

Ultrasonic speed

Assessment of speed of sound through theoretical calculation in liquid combinations and its connection to interaction has been effectively applied in recent times. Acoustic speeds in combinations have been calculated and compared with investigational values using various theories. Such estimation proposes an easy means to probe molecular interactions as properly to validate the applicability of different theories to binaries. Acoustic speed worked out through a variety of relations along with investigational values at 308.15 K is exposed in Fig S1 of Supplementary file. From the observed curves, a fine concurrence among theoretical and experimental values is observed for Nomoto relation. Variations among evaluated and investigational values are not only due to interactions occurring among the heteromolecules but also the limitations and approximation incorporated in these theories.

Table 11 Computed derivatives of thermodynamic potentials ($H_m/S_m/G_m/\alpha_P/P/T$ are enthalpy/entropy/Gibb's free energy/thermal expansion coefficient/pressure/temperature, respectively) at T = (308.15/313.15/318.15) K

x_1	$\left(\frac{\partial^2 G_m}{\partial P \partial T}\right)/10^{-7}$ J/Pa K mol	$\left(\frac{\partial S_m^E}{\partial P}\right)_T/10^{-8}$ J/K mol Pa	$\left(\frac{\partial S_m}{\partial P}\right)_T/10^{-7}$ J/mol K Pa	$\left(\frac{\partial^2 V}{\partial T^2}\right)_P/10^{-10}$ J/mol Pa K^2	$\left(\frac{\partial^2 H_m}{\partial P^2}\right)_S/10^{-14}$ J/mol Pa^2	$\left(\frac{\partial^2 G_m}{\partial P^2}\right)_T/10^{-14}$ J/Pa^2 mol	$\left(\frac{\partial \alpha_P}{\partial T}\right)_P/10^{-6}$ K^{-2}
T = 308.15 K							
0.0000	1.0888	0.0000	− 1.0888	0.9801	− 6.1159	− 8.3749	− 2.7538
0.1137	1.0986	0.1497	− 1.0986	− 17.6428	− 6.0330	− 8.2373	18.0323
0.2134	1.1085	0.2676	− 1.1085	− 32.0546	− 5.9849	− 8.1505	32.5344
0.3343	1.1232	0.3844	− 1.1232	− 46.5478	− 5.9553	− 8.0877	45.5103
0.4321	1.1378	0.4514	− 1.1378	− 55.4169	− 5.9533	− 8.0715	52.3261
0.5023	1.1505	0.4768	− 1.1505	− 60.0861	− 5.9635	− 8.0809	55.2972
0.6111	1.1739	0.4805	− 1.1739	− 63.9621	− 5.9983	− 8.1283	56.5509
0.7432	1.2094	0.4126	− 1.2094	− 62.6835	− 6.0715	− 8.2439	52.7742
0.8331	1.2387	0.3155	− 1.2387	− 57.5816	− 6.1410	− 8.3606	46.8620
0.9112	1.2684	0.1893	− 1.2684	− 50.1578	− 6.2146	− 8.4903	39.5818
1.0000	1.3066	0.0000	− 1.3066	− 38.0113	− 6.3138	− 8.6697	28.8341
T = 313.15 K							
0.0000	1.1077	0.0000	− 1.1077	0.9927	− 6.4304	− 8.7892	− 2.7965
0.1137	1.0222	0.8770	− 1.0222	− 17.8504	− 6.3299	− 8.2561	18.3595
0.2134	0.9586	1.5326	− 0.9586	− 32.4062	− 6.2700	− 7.9050	33.0778
0.3343	0.8995	2.1476	− 0.8995	− 47.0224	− 6.2299	− 7.6112	46.2134
0.4321	0.8690	2.4713	− 0.8690	− 55.9558	− 6.2223	− 7.4708	53.0957
0.5023	0.8581	2.5941	− 0.8581	− 60.6550	− 6.2299	− 7.4202	56.0886
0.6111	0.8619	2.5777	− 0.8619	− 64.5509	− 6.2631	− 7.4238	57.3375
0.7432	0.9042	2.1810	− 0.9042	− 63.2543	− 6.3380	− 7.5657	53.5005
0.8331	0.9595	1.6449	− 0.9595	− 58.1099	− 6.4110	− 7.7580	47.5122
0.9112	1.0271	0.9849	− 1.0271	− 50.6255	− 6.4893	− 7.9987	40.1408
1.0000	1.1273	0.0000	− 1.1273	− 38.3761	− 6.5959	− 8.3701	29.2545
T = 313.15 K							
0.0000	1.1271	0.0000	− 1.1271	1.0056	− 6.7637	− 9.2433	− 2.8403
0.1137	0.9431	1.6310	− 0.9431	− 18.0437	− 6.6393	− 8.3030	18.6650
0.2134	0.8040	2.8383	− 0.8040	− 32.7075	− 6.5627	− 7.7293	33.5442
0.3343	0.6696	3.9596	− 0.6696	− 47.3923	− 6.5073	− 7.2833	46.7622
0.4321	0.5934	4.5415	− 0.5934	− 56.3501	− 6.4908	− 7.0808	53.6598
0.5023	0.5585	4.7610	− 0.5585	− 61.0578	− 6.4940	− 7.0048	56.6498
0.6111	0.5426	4.7206	− 0.5426	− 64.9587	− 6.5231	− 6.9889	57.8830
0.7432	0.5917	3.9863	− 0.5917	− 63.6598	− 6.5978	− 7.1299	54.0172
0.8331	0.6735	3.0021	− 0.6735	− 58.5040	− 6.6736	− 7.3452	47.9979
0.9112	0.7796	1.7977	− 0.7796	− 50.9952	− 6.7562	− 7.6361	40.5832
1.0000	0.9430	0.0000	− 0.9430	− 38.6877	− 6.8699	− 8.1257	29.6143

Nonlinearity parameter $\left[\frac{B}{A}\right]$

The nonlinearity parameter $\left[\frac{B}{A}\right]$ of a fluid is a fundamental property which decides deformation of a restricted signal while transmitting in liquid. This is not only linked to the kinematics of the channel but also impart sources concerning properties pertinent to structure of channel, intrinsic pressures, gathering and intermolecular gaps. Significance of $\left[\frac{B}{A}\right]$ escalate with the growth of elevated-pressure expertise of groceries dispensation and conservation. Here, an effort has made to work out on molecular properties of the combinations from empirical equations derived by *Hartmann–Balizar (H&B)* [73] and *Ballou* [74] by the employ of Sehgal's equations [75] at all temperatures in study. Excess $\left[\frac{B}{A}\right]$ are found to be negative and emphasise prevalence of strong interaction among hetero

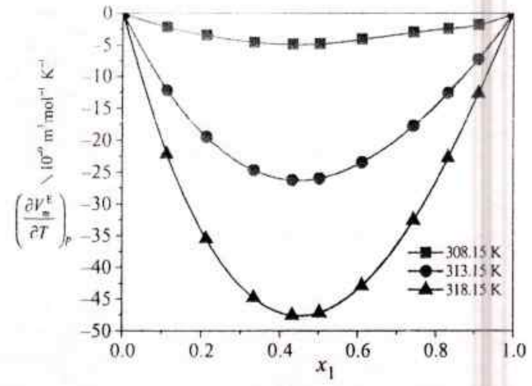

Fig. 7 Plots of $\left(\frac{\partial V_m^E}{\partial T}\right)_P$ against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

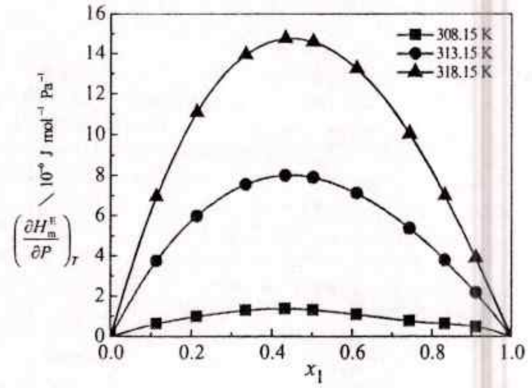

Fig. 8 Plots of $\left(\frac{\partial H_m^E}{\partial P}\right)_T$ against mole fraction (x_1) of MB in the mixture with DMC at different temperatures

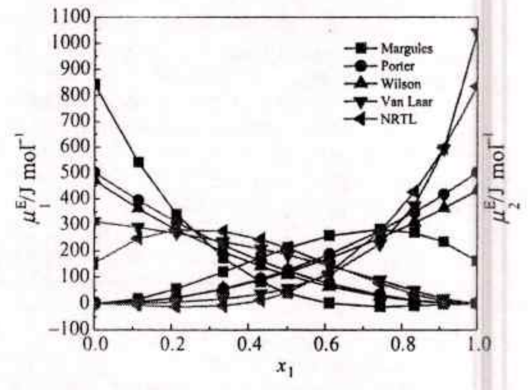

Fig. 9 Variation of excess chemical potentials μ_1^E (MB) and μ_2^E (DMC) with mole fraction, x_1 computed from Margules, Porter, Wilson, Van Laar and NRTL at $T = 308.15$ K

molecules [6]. Additional evaluated molecular properties from nonlinear parameter are shown in Supplementary file of Table S2.

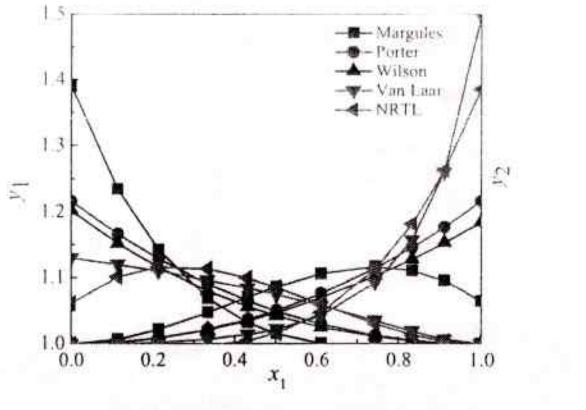

Fig. 10 Variation of activity coefficients y_1 (MB) and y_2 (DMC) with mole fraction, x_1 computed from Margules, Porter, Wilson, Van Laar and NRTL at $T = 308.15$ K

Conclusions

1. To investigate molecular interactions, the density/speed of sound data of (dimethyl carbonate (2) + methyl benzoate (1)) has been used to compute V_m^E, $\overline{V}_m^E$, $\overline{V}_m^{E,\infty}$, κ_s^E, partial/excess molar compressibilities, $\boldsymbol{n}$, $\boldsymbol{R_A}$, κ_T^E, L_f^E, Z^E, u^E. The sign/magnitude of these parameters with composition/temperature emphasised dominance of strong interactions (dipole–dipole interactions + molecular fitting due to difference of molar volume) and its rise to follow: (318.15 > 313.15 > 308.15) K.
2. At $T = 308.15$ K, correlation is made between experimental and evaluated V_m^E through PFP/topology theories, cubic equation of states of Soave–Redlich–Kwong (SRK)/Peng–Robinson (PR). Moreover, thermodynamic potential derivatives are computed. Additionally, evaluation and correlation is made for excess chemical potential/activity coefficients/ultrasonic speed by semi-empirical relation.
3. Molecular properties are computed through Sehgal's relations on nonlinear equations at all T.

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