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Study of Molecular Interactions of Fossil Fuels through Acoustic and Volumetric Data

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Densities and speeds of sound of binary mixtures formed by Diethyl carbonate (DEC) with isomeric methyl phenols (2/3/4) were measured over the entire mole fraction range at 303.15 to 318.15 K at atmospheric pressure. Employing these, several excess properties *viz*., excess molar volume, V_m^E, excess speed of sound, u^E, excess isentropic compressibility, k_S^E, excess molar isentropic compressibility, $K_{s,m}^E$, and excess isobaric thermal expansion, α_p^E, of the binary systems were calculated. To better understand the solute and solvent interactions, excess partial molar volumes, $\overline{V}_{m,1}^E$ and $\overline{V}_{m,2}^E$, and excess partial molar volumes, $\overline{V}^{0E}_{m,1}$ and $\overline{V}^{0E}_{m,2}$ of the components at infinite dilution were also measured. The excess parameters were subjected to fitting using the Redlich-Kister polynomial equation. The findings were analysed to investigate the prevalent molecular interactions and their consequence on the structural aspects.

Keywords: DEC, Methyl phenol, Isentropic compressibility, Excess functions, Partial molar properties

INTRODUCTION

Volumetric properties of binary combinations and their familiarity with composition and temperature dependence provide significant information on the molecular effect on the strength of intermolecular interactions between component molecules [1]. The knowledge of the physicochemical properties of liquids and their mixtures plays a wide role in theoretical and industrial research. The outcomes are generally used in design processes such as flow, mass, or heat transfer calculations in industries such as chemical, textile, leather, and nuclear industries. Volumetric and acoustic properties of liquids and the combinations are important to analyse the molecular interactions and other factors such as size, shape, packing effect, *etc*. [2,3]

The energy situation for the past many years is focused on expanding the utilization of biofuels, particularly the ones that evolve through rural and modern waste, *viz*., second generation biofuels. As per the World Energy Committee, these biofuels will approximately contribute 40% of all vehicle fluid energies by 2050. In recent times, biofuels have started to exhibit their dominance and their utilization is required to quickly extend all through the world. So, it gives more interest to authors to choose the combination of these molecules.

The present paper is the continuation of our previous investigations of Diethyl Carbonate (DEC) [4] with methyl phenols [5]. DEC, an ester, is primarily employed as solvent in pharmaceutical applications and batteries as electrolytes [6]. It shows strong potential as fuel additive (40.6% of oxygen by mass) to help greener diesel combustion process owing to its high boiling point that may reduce fuel volatility leading to minimal vapour build-up [7]. In addition, they are also industrially relevant in the form of petrol additives and as lubricants with the novel HFCs. The

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isomeric methyl phenols are also used extensively as precursors, for materials like pyrethroid insecticides and pharmaceutical products, *viz*., is infectants, fungicides, bactericides, wood preservatives, local antiseptics, parasiticides [8], dyes, and in manufacturing carbon nanotubes. The 3- and 4-isomers are extensively used for manufacture of phenol-formaldehyde resins [9].

The combination of DEC with isomeric methyl phenols plays a vital role in the pharmaceutical as well as petroleum industry as supplant of fossil fuels. The aim of the present study is to investigate the nature and extent of intermolecular interactions through the experimentally determined properties and their excess counterparts with their signs brought about by change in the position of -OH group in isomeric methyl phenols with DEC.

This work investigates the density, ρ, speed of sound, u-, isobaric thermal expansivity, α_p, excess properties of molar volume, V_m, isentropic compressibility, κ_s, molar isentropic compressibility, $K_{s,m}$, speed of sound, u, isobaric thermal expansion, α_p, and excess partial molar volumes, $\overline{V}_{m,i}^{E,\infty}$, at infinite dilution for the isomeric methyl phenols with DEC at 303.15 to 318.15 K over the entire mole fraction range at atmospheric pressure.

MATERIALS AND METHODS

The compound names, their sources of purchase, and supplier purities of the components used in this experiment have been compiled in Table 1. Before the preparation of solutions, all the components were degassed by ultrasound technique to minimize the measurement errors. The methyl phenols and DEC (Sigma-Aldrich, USA, mass fraction purity 0.99) have been purified using standard methods. Karl Fischer titrator (890 KF Titrando, Metrohm, USA) was used to measure the water content in the chemicals and summarized in Table 1.

The preparations of the samples were carried out just prior to the measurements with an electronic balance (CPA-225D, Sartorius, Germany) capable of measuring precisely within ± 1 × 10^{-5} g. The mole fraction uncertainty was found to be within ± 1 × 10^{-4}.

Density measurements were carried out using a single-capillary pycnometer (Borosil-bulb capacity of ≈10 ml). The capillary, with graduated marks, had a uniform bore and could be closed by a well-fitting glass cap. Use was made of triple distilled water to calibrate the graduations on the pycnometer and the density values of pure water compared that from literature with the reproducibility seen to be within ± 1 kg m^{-3}. The speeds of sound were measured by a variable-path, single-crystal multi-frequency ultrasonic interferometer (F-81, Mittal Enterprises, India) working at 2 MHz and was found to be reproducible within ± 0.8 m s^{-1}. Temperature measurements were carried out using a Julabo (FT 200, Julabo Labortechnik, Gmbh, Germany) thermostatic bath having an accuracy of ±0.02 K. A self-optimizing electronic PID-control circuit automatically

Table 1. Details of Studied Compounds, CAS Number, Source, Purification Method, Purity, and Analysis Method

Chemical name	CAS number	Source	Initial mole fraction purity	Purification method	Final water mass Fractionb	Final mole fraction purity	Analysis method[a]
Diethyl carbonate	105-58-8	Sigma Aldrich	0.99	Fractional distillation	$< 5 \cdot 10^{-4}$	0.993	GC
o-cresol	95-48-7	Sigma Aldrich	0.99	Fractional distillation	$< 2 \cdot 10^{-4}$	0.993	GC
m-cresol	108-39-4	Sigma Aldrich	0.99	Fractional distillation	$< 2 \cdot 10^{-4}$	0.993	GC
p-cresol	106-44-5	Sigma Aldrich	0.99	Fractional distillation	$< 2 \cdot 10^{-4}$	0.993	GC

[a]GC = Gas chromatography. [b]KF Titration.

adjusts the heat supply to the value required by the bath and pressure was kept at ambient.

In the present paper, 4-methyl phenol density and speed of sound values are a little bit varies from our previous paper [5] and the variation agrees, except for the speed of sound data at 318.15 K. Authors noticed the discrepancy in our previous work [5] due to typographical mistake [5,21] instead of 1423.1 m s^{-1} it was typed as 1433.1 m s^{-1}.

AAD (average absolute deviation) has been used to carry out a comparative study [10-27] of the densities and speeds of sound of DEC with $AAD = (100/n)\sum_{i=1}^{n}(F_{0,lit} - F_{0,exp}/F_{0,lit})_i$ and reported in Table 1S. The maximum deviation of DEC density is ± 0.03% and the speed of sound is -0.08%. This discrepancy may be due to impurities of chemicals or experimental procedures. Whereas all methyl phenols density is in limits of -1.0 to +0.3% and speed of sound is +0.56 to -0.09%.

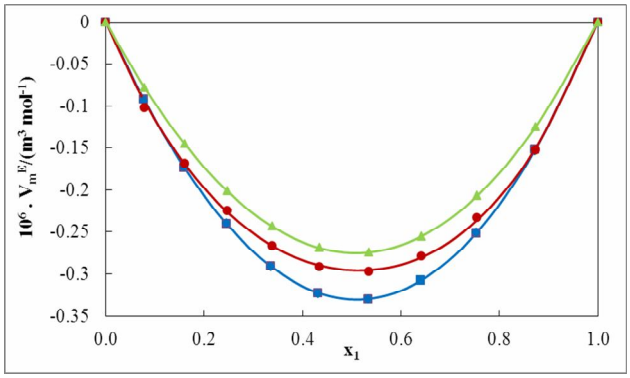

Fig. 1. Variation of excess molar volume (V_m^E) with mole fraction x_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (■), *o*-cresol; (●), *m*-cresol; (▲), *p*-cresol; at T = 303.15 K. The points represent experimental values and solid lines have been drawn from R-K equation using the coefficients given in Table 3S.

THEORY

All the formulas related to this manuscript are in the supplementary file.

DISCUSSION

The comparison of excess molar volumes, V_m^E, of all binary mixtures at T = 303.15 K was depicted in Fig. 1. The V_m^E values are observed to be negative over the whole composition range. The minima were observed at 0.5 mole fraction for all DEC with 2/3/and 4-methyl phenol binary mixtures.

The sign and magnitude of excess functions that result in component mixing are the result of numerous factors that might operate in the same or opposite direction [32].

The negative contributions can be arising due to the consequence of (a) formation of strong molecular interactions attributed to the ion-dipole, dipole-dipole, charge transfer (donor-acceptor) complexes, or hydrogen bonding, *etc*. among distinct molecules (b) structural contributions are due to interstitials geometric fitting of molecules of the other component.

The excess molar volume, V_m^E, values for all the binary systems become more negative with increasing temperature. A subjective explanation can offer for these results *i.e*., H-bonding and packing create interstitial spaces that can be filled by smaller molecules [17]. Out of these two factors, hydrogen bond interaction is the most dominant factor. DEC is a non-polar solvent and the diffusion of a solvated electron in this kind of solvent is very fast. The solvation energy of the electron in a non-polar solvent is low and the electron can move from one cavity to another one very quickly. Therefore, the electron can be very speedily trapped by methyl phenol molecules. It can be attributed to more vital dispersion forces or considering the breakage of intermolecular interactions dipole-dipole in the carbonate group and forms new bonds with methyl phenols, *i.e*., interaction parameters corresponding to the carbonate group of the type (-OCOO-) with a phenolic group (-OH) of the methyl phenols [16] are increased leading to a more significant contraction in the mixture volumes with increasing temperature [33]. For all the binaries, with rise of temperature, a significant increase in V_m^E values noticed. The depth and position of the minima are dependent on the degree of connection as well as the shape of the molecules, (*i.e*., the position of methyl group) as shown in Fig. 1. This was attributed to the fact that the 2-methyl phenols are

clearly less self-associated than either 3- or 4-methyl phenols in their pure state. As a result, the highest negative excess molar volume can be obtained in 2-methyl phenol mixes resulted in the creation of multimer species, that decreased the average degree of cross-association mixtures of 2-methyl phenol with the other two isomers [25]. The absolute V_m^E values have been observed in the following order: 2-methyl phenol > 3-methyl phenol > 4-methyl phenol.

Benzyl alcohol, 1,4-butanediol, and β-pinene were followed by methyl phenols in the same order [5,34,35]. The same trend has not been observed for 2-methoxyaniline with methyl phenols & ethanoic acid/propanoic acid/ butanoic acid with methyl phenols [36].

At 303.15 K, the findings of κ_s^E and u^E for all three systems are shown in Figs. 2 and 3. According to the findings of this study, κ_s^E and u^E are opposite in trend for all systems over the DEC concentration. The molecular interactions that govern the behaviour of these combinations can be explained. u^E value can be read as dipole-dipole interactions, charge transfer complex, and phenol component takes interstitial accommodation in the DEC lattice. The hydroxyl ion on phenol affects the physical and chemical properties of the benzene ring. New intermolecular interactions are formed due to the hydroxyl ion on phenol enhances the more electron concentration around the internuclear axis on the ring. As a result, there are fewer interspaces between molecules in mixtures, resulting in negative compressibility deviations.

The excess molar isentropic compressibility, $K_{s,m}^E$, *vs*. DEC (x_1), presented (Fig. 4) at 303.15 K. Over the entire mole fraction range, the $K_{s,m}^E$ values for all three binary liquid combinations are negative, as shown in the figure. Negative $K_{s,m}^E$ values reveal that these binary mixtures are less compressible than their ideal mixtures. As a result, in these instances, free volume contraction occurs, making the mixture less compressible than the ideal mixture, resulting in negative values of $K_{s,m}^E$, resulting in increased intermolecular contact. The sequence of $K_{s,m}^E$ as follows: 2-methyl phenol > 3-methyl phenol > 4-methyl phenol. This could be related to steric considerations; the aqueous affinity of 2-methyl phenol (hindered hydroxyl group) is expected to be lower than 3- and 4-methyl phenol (unhindered), owing to the methyl group's close proximity to the active hydroxyl functionality. As a result, the total charge transfer complex in 4-methyl phenol is lower than in 3- and 2-methyl phenol.

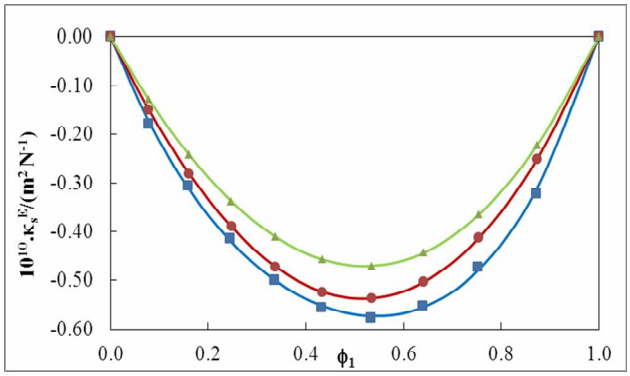

Fig. 2. Excess isentropic compressibility (κ_s^E) with volume fraction ϕ_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (■), o-cresol; (●), m-cresol; (▲), *p*-cresol; at T = 303.15 K. The points represent experimental values and solid lines have been drawn from R-K equation using the coefficients given in Table 3S.

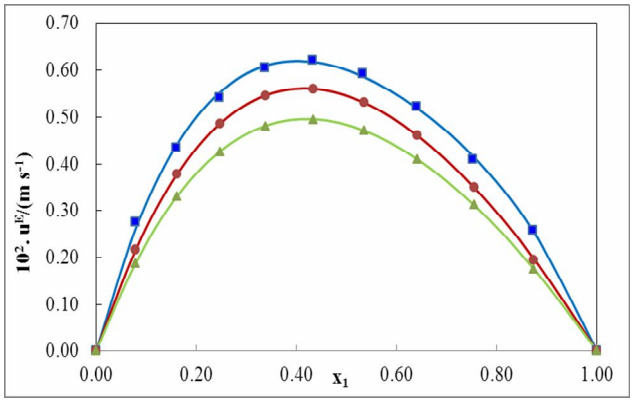

Fig. 3. Excess speed of sound (u^E) with mole fraction x_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (■), *o*-cresol; (●), *m*-cresol; (▲), *p*-cresol; at T = 303.15 K. The points represent experimental values and solid lines have been drawn from R-K equation using the coefficients given in Table 3S.

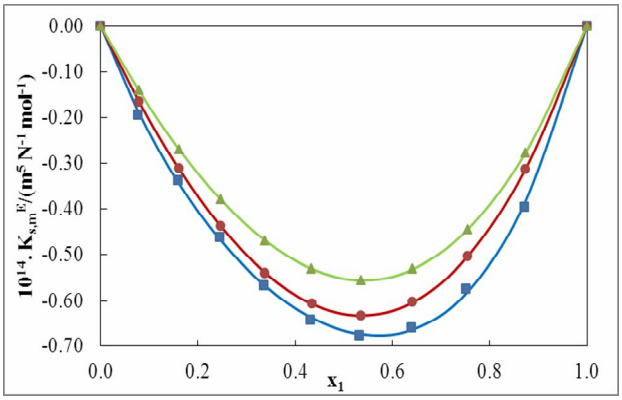

Fig. 4. Excess molar isentropic compressibility ($K_{s,m}^{E}$) with mole fraction x_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (■), *o*-cresol; (●), *m*-cresol; (▲), *p*-cresol; at T = 303.15 K. The points represent experimental values and solid lines have been drawn from R-K equation using the coefficients given in Table 3S.

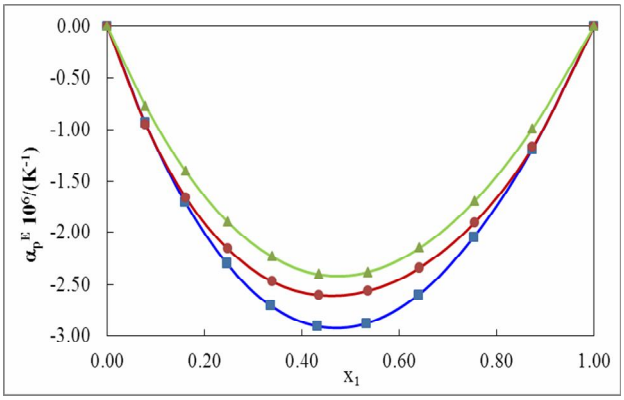

Fig. 5. Excess isobaric thermal expansion (α_p^E) with mole fraction x_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (■), *o*-cresol; (●), *m*-cresol; (▲), *p*-cresol; at T = 303.15 K. The points represent experimental values and solid lines have been drawn from the R-K equation using the coefficients given in Table 3S.

The plot of u^E *vs*. the mole fraction of DEC (Fig. 3) reveals that the u^E values are all positive over the full range of composition, with the maxima deviation observed at x_1 = 0.5 of the first component. It's also clear that as the temperature rises, the deviation decreases, with the maxima deviations occurring at the lower end of the temperature range, 303.15 K. Furthermore, the speed of sound values decreases as the mole of fraction increases from 0 to 1. According to Eyring [37], a decrease in sound velocity occurs during mixing, resulting in an increase in intermolecular free length [17] and possibly a reduction in excess isentropic compressibility. All excess speed of sound values shows a similar trend for all binary mixtures and support the excess molar volume V_m^E.

Table 2S lists the isobaric thermal expansivity α_p^E of pure DEC and methyl phenol molecules, and values are shown graphically as a function of DEC at 303.15 K in Fig. 5.

Isobaric thermal expansions are calculated for each composition for a better understanding of the structure of the solution in mixing process. In addition, as the temperature rises, the curves maxima increase. This behaviour is like that observed for other excess volumetric properties of binary systems, such as excess volume or excess isothermal compressibility. Packing effects, hydrogen bond breaking, and dissimilarities in dispersion forces between like and unlike molecules are used to explain these findings. The accommodation of methyl phenol molecules in the hydrogen-bonded structure of DEC methyl phenols causes packing effects. This could be owing to significant interactions between the mixture's dissimilar molecules [38].

Partial Molar Properties

The values of partial molar properties, $\overline{V}_{m,1}^{\circ}$ and $\overline{V}_{m,2}^{\circ}$, $\overline{K}_{s,m,1}^{\circ}$ and $\overline{K}_{s,m,2}^{\circ}$, of DEC and methyl phenols at infinite dilution were calculated by using the Eqs. (20) nd (21), and the excess partial molar properties, $\overline{V}_{m,1}^{\circ E}$ and $\overline{V}_{m,2}^{\circ E}$, $\overline{K}_{s,m,1}^{\circ E}$ and $\overline{K}_{s,m,2}^{\circ E}$ at infinite dilution were calculated using the Eqs. (22) and (23) by substituting $\overline{V}_{m,1}^{\circ E}$ and $\overline{V}_{m,2}^{\circ}$, $\overline{K}_{s,m,1}^{\circ E}$ and $\overline{K}_{s,m,2}^{\circ E}$ in place of $\overline{V}_{m,1}^{E}$ and $\overline{V}_{m,2}$, $\overline{K}_{s,m,1}^{E}$ and $\overline{K}_{s,m,2}^{E}$, respectively. The values of $\overline{V}_{m,1}^{\circ}$, $V_{m,1}^{*}$, $\overline{V}_{m,1}^{\circ E}$, $\overline{V}_{m,2}^{\circ}$, $V_{m,2}^{*}$ and $\overline{V}_{m,2}^{\circ E}$ & $\overline{K}_{s,m,1}^{\circ}$, $K_{s,m,1}^{*}$, $\overline{K}_{s,m,1}^{\circ E}$, $\overline{K}_{s,m,2}^{\circ}$, $K_{s,m,2}^{*}$, $\overline{K}_{s,m,2}^{\circ E}$ for the binary mixtures at each investigated temperature are listed in Tables 4S and 5S.

As a function of mole fraction, x_1 of DEC and temperature, the values of $\bar{V}_{m,1}$, $\bar{V}_{m,2}$, $\bar{V}^E_{m,1}$, $\bar{V}^E_{m,2}$ and $\bar{K}_{s,m,1}$, $\bar{K}_{s,m,2}$, $\bar{K}^E_{s,m,1}$, and $\bar{K}^E_{s,m,2}$ have been given in Tables 6S and 7S and the variations of $\bar{V}^E_{m,1}$, and $\bar{V}^E_{m,2}$ & $\bar{K}^E_{s,m,1}$, and $\bar{K}^E_{s,m,2}$ with composition at 303.15 K are presented in Figs. 6 and 7.

A thorough examination of the values of $\bar{V}^E_{m,1}$, and $\bar{V}^E_{m,2}$ & $\bar{K}^E_{s,m,1}$, and $\bar{K}^E_{s,m,2}$ Figs. 6 and 7 reveals that they are all negative for the three binary mixtures over the entire composition range. By this, the molar volumes of each component in the binary combination are fewer than their respective molar volumes in the pure state, implying that when DEC is mixed with methyl phenols, the volume decreases. The negative $\bar{V}^E_{m,1}$ and $\bar{V}^E_{m,2}$ & $\bar{K}^E_{s,m,1}$ and $\bar{K}^E_{s,m,2}$ values, in general, indicate that there are considerable solute-solvent interactions between dissimilar molecules [39] in the mixture. The DEC-DEC or methyl phenols-methyl phenols interactions are smaller than the DEC-methyl phenols interactions, as seen by the negative $\bar{V}^E_{m,1}$, and $\bar{V}^E_{m,2}$ & $\bar{K}^E_{s,m,1}$, and $\bar{K}^E_{s,m,2}$ values.

A closer study in Tables 4S & 5S demonstrates that at each temperature tested the values of $\bar{V}^{0,E}_{m,1}$ and $\bar{V}^{0,E}_{m,2}$ & $\bar{K}^{\circ E}_{\mathrm{s,m,1}}$ and $\bar{K}^{\circ E}_{\mathrm{s,m,2}}$ are negative for three binary systems. This indicates that each component's molar volume in a mixture is in pure condition less than the corresponding molar volume, *i.e.* the combining of DEC and methyl phenols results in volume contracture. Negative excessive volumes of molar ingredients ($\bar{V}^{0,E}_{m,1}$ and $\bar{V}^{0,E}_{m,2}$ & $\bar{K}^{\circ E}_{\mathrm{s,m,1}}$ and $\bar{K}^{\circ E}_{\mathrm{s,m,2}}$) can be viewed as a sign of novel interactions with molecular systems or as a consequence of interstitial accommodation, or as a symptom of the incorporation into DEC cavities of methyl phenols [40]. Clathrate forming should be strongly linked to a solution fit into solvent structures, with the relative size of the co-solvents. This effect was determined in combinations of DEC-methyl phenol.

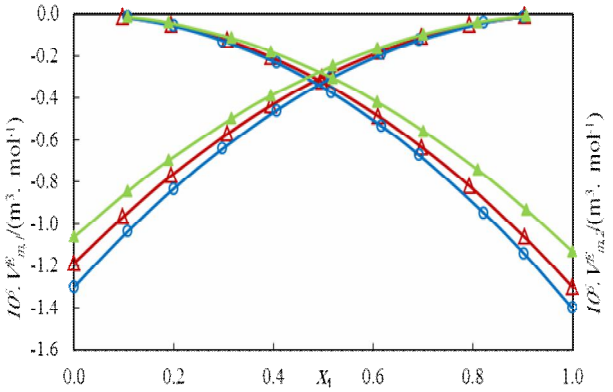

Fig. 6. Excess partial molar volume ($\bar{V}^E_{m,1}$ and $\bar{V}^E_{m,2}$) with mole fraction x_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (o), *o*-cresol; (Δ), *m*-cresol; (▲), *p*-cresol; at T = 303.15 K.

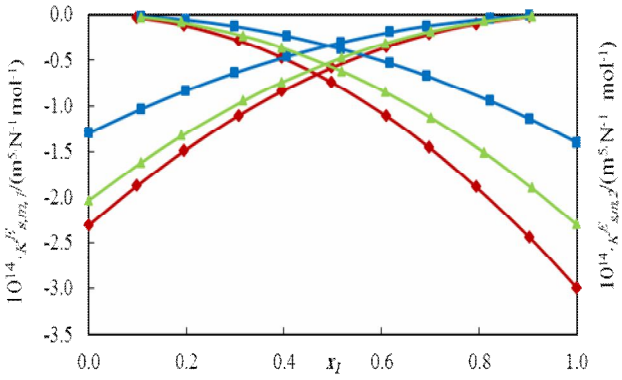

Fig. 7. Excess partial molar compressibility ($\bar{K}^{\mathrm{E}}_{\mathrm{s,m,1}}$ and $\bar{K}^{\mathrm{E}}_{\mathrm{s,m,2}}$) with mole fraction x_1 of DEC in the binary mixtures of DEC (1) with cresols (2); (■), *o*-cresol; (♦), *m*-cresol; (▲), *p*-cresol; at T = 303.15 K.

CONCLUSIONS

In the present article, the density and speed of sound of binary mixtures of DEC with 2-/3-&4-methyl phenol had measured for all compositions at temperatures 303.15, 308.15, 313.15, and 318.15 K. Negative values are observed for excess molar volume, isentropic compressibility, and molar isentropic compressibility of binary liquid mixtures of DEC with 2, 3 and 4 methyl phenols over the whole composition range. The results are analysed in terms of specific interactions through the attractive force of interactions between the components of the mixtures, resulting in the formation of associated complexes via donor-acceptor interactions, and are arranged in the following order: 2-methyl phenol > 3-methyl phenol > 4-methyl phenol.

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