Indian Journal of Chemistry
Vol. 64, July 2025, pp. 682-687
DOI: 10.56042/ijc.v64i7.13304

Effect of role of industrially important solvents on excess thermodynamic functions of non-electrolyte solutions

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Received 21 August 2024; accepted (revised) 24 June 2025

The density (ρ) with displacements (u) for mixtures of binary compounds containing 1,3-dichlorobenzene containing *o*-, *m*-, and *p*-cresol have been experimentally determined and has an expression within the temperature span of 303.15, 308.15 and 313.15K in addition to over the entire mixture span. The evaluation for all aqueous integrates has been utilized for calculating surplus volumes (V^E), surplus isotropic compressibility (Ks^E), along with isotropic compressible material (Ks). The Redlich-Kister expression has been fitted using the estimated surplus variables. The outcomes have been studied in the light of chemical mechanisms and structural implications among individual compounds. Various theoretical models have been employed for evaluating the obtained aqueous integrates based on noise data, particularly a collision aspect hypothesis. For identical configurations, compressibilities and surplus fractional molecular quantities have been evaluated.

Keywords: Binary integrating, Surplus attributes, Theory, Accident variables, 1,3-Dichlorobenzene, *o*-, *m*-, and *p*-cresol

The thermophysical qualities of combinations, for instance the combination that includes organic fluids with cresols, have significance from a technological and scientific viewpoint perspective[1,2]. A greater awareness regarding something less than perfect behaviors in a binary mechanism also calls for a comprehension of the essential thermodynamics attributes of fluid mixtures owing to their chemical and physical impacts that occur within molecular interactions, intermolecular motion, as well as additional conditions across *versus* molecules of matter. The thermodynamic characteristics were effectively vital for the sophisticated estimate for various thermodynamic simulations needed for most effective activities for the chemical-based, petrochemical manufacturing, medicinal products as well as various other sectors. More comprehensive information presenting the fundamental characteristics associated with fluid combinations must be collected for the purpose to formulate predictions involving fluid phases. Incredibly widely acknowledged how the formulation including assessment of numerous response hypotheses and mathematical representations depend heavily on knowledge of the interactions between molecules within components of liquids[3]. These characteristics comprise surplus isotropic the compressibility as well as surplus quantity. There are several potential uses for the liquids chosen for this investigation throughout the chemical industry. Cresols are among there are several significant classes for substances that are aromatic in nature. They are used in the manufacture of various phenol resins, organic intermediates as well, fabric scrubbing representatives, chemical herbicides, coumarin, which or tri crysyl phosphate, amongst other materials[4,5]. Moreover, cresols are a byproduct of the production of azo pigments and Lysol and Creosote, among the more frequently utilized compounds[6]. Thermodynamic properties of liquid solutions, such as cresols and various solvents made from organic substances were documented. The current work examines self-association by intra- and intermolecular bonding of hydrogen *via* isomeric cresols in mixtures of 1,3-dichlorobenzene[7,8]. The current work attempts to elucidate the characteristics of molecular interactions among 1,3 dichlorobenzene as well as cresols through measurements of capacities (ρ) from 303.15 K to 323.15 K through noise accelerates (u) at 303.15 K and

313.15 K. Furthermore, the collected sound velocity information can be evaluated by making use of Schaff's collision impact concept[9-13]. The goal of the present study sought to investigate if adding a –OH group to the toluene component or changing therefore *ortho*, *meta*, and *para* locations would have any impact upon the magnitude and intensity of the surplus thermodynamic parameters given the aforementioned binary schemes.

Experimental Section

Computational and Experimental Methods

Materials

The substances utilized throughout this existing endeavor are through Indian S.D. Fine Chemical Limited., and they are of A.R. grade. Each liquid had been dried employing 0.4 nm pore sizes after the fractional distillation process, in accordance with protocols from previous studies, before experimental findings were made[14]. Gas chromatography is used to look at fractions of mass purities, and Analab (Micro Aqua Cal 100) Karl Fischer Titrator was utilized to investigate the level of humidity in the fluids employed for the present investigation. Table 1 illustrates the outcomes. Furthermore, reported values for T=303.15K to 323.15K were contrasted to the witnessed concentrations and noise velocity; the outcomes indicated that they are consistent and are presented in Table 2. This enabled it practicable for confirming the substances integrity.

Measurements

With the objective to prevent excessive humidity percentage and vaporization, 1,3-dichlorobenzene and cresol combinations can be made by syringing every constituent towards a tightly sealed obstruction container. The right quantity of pure fluids is subsequently Utilizing a digital instrument weighing device (Afoset, ER-120A, India) with a precise measurement of ± 0.1 mg. The predicted value regarding the fraction of moles had been apart approximately ±1×10-4. Whenever the specimen has been mixed, the homogeneous, free of bubbles solution is introduced directly into the U-tube of the densimeter using an injector. The concentrations have been determined using a Rudolph Research Analytical digital densimeter (DDH-2911 Model). The accuracy in fluid integrates utilized to estimate the density is $\pm 2\times10^{-3}$ gcm^{-3} (Ref. 15,16). A multifrequency acoustic spectrometer (M-82 Model, Mittal Enterprise, New Delhi, India) running at 2 MHz is used to calculate the velocity of sound waves for binary combinations of liquids at 303.15 K and 313.15 K employing an electronic stable temperature immersion water bath. The noise caused by velocity measuring inaccuracy amounts to approximately 0.3%. Its temperature consistency is retained within ± 0.02 K by means of a water bath with a thermostat that is pumped throughout each cell by a revolving compressor.

The functioning of the rangefinder has been evaluated by contrasting the calculated velocity of sound of an isomeric cresols and pure isolates of 1,3-dichlorobenzene, whose measurements are quite consistent with the reported specifications[17-30] at T=303.15K. Table 2 summarizes the results of this study.

Results and Discussion

Excess volumes *(VE)*

Based on the scientifically developed the density statistics, the additional molar proportions (VE) of binary sequences of 1, 3-dichlorobenzene cresols that are isomeric measured utilizing the subsequent equation:

$$V^E/cm^3.mol^{-1} = [[X_1 M_1 + X_2 M_2]/\rho_m - [X_1 M_1/\rho_1 + X_2 M_2/\rho_2]] \quad \ldots(1)$$

In this case, ρ_m is the measured mixture density while X_1, X_2, M_1, M_2, ρ_1 and ρ_2 refer for the mole portion, molar quantity, as well as percentage of the individual parts 1 and 2, correspondingly.

Table 1 — Name of the chemical, source, CAS number, purity in mass fraction, purity analysis method and water content in mass fraction of the chemicals used in this work

Component	Source	CAS number	Purity in mass fraction (as received from supplier	Purity in mass fraction (after purification)	Analysis method*	Water content in mass fraction
1,3-Dichlorobenzene	S.D.Fine Chemicals. Ltd.		0.995	0.996	GC	0.0004
o-Cresol	S.D.Fine Chemicals. Ltd.	95-48-7	0.99	0.993	GC	0.0006
m-Cresol	S.D.Fine Chemicals. Ltd.	108-39-4	0.98	0.994	GC	0.0006
p-Cresol	S.D.Fine Chemicals. Ltd.	106-44-5	0.985	0.995	GC	0.0007

*GC=Gas Chromatography

Table 2 — Density (ρ) and sound speed (u) values for the pure components along with literature values at temperatures studied and at 0.1 MPa pressure

T/K	ρ/(gcm^3)		u/(ms^{-1})	
	Exp.	Lit.	Exp.	Lit.
		1,3-diChlorobenzene		
303.15	1.28899	1.28922	1256	1255 1249
308.15	1.28642	1.28735	–	1248
313.15	1.28482	1.28442	1253	1254.8
318.15	1.28220	–	–	1246
323.15	1.28056	–	–	–
		o-cresol		
303.15	1.03651	1.037046 1.0369	1488	1488.19 1487
308.15	1.03212	1.032642 1.03273	–	–
313.15	1.02779	1.028145 1.0282	1452	1452.65 1452.11
318.15	1.02336	1.023825 1.0211	–	–
323.15	1.01895	1.019387 1.0198	–	–
		m-cresol		
303.15	1.02406	1.025959 1.0261	1466.21	1466.16 1465
308.15	1.02008	1.021988 1.0215	–	–
313.15	1.01605	1.0170 1.01763	1438	1439.97 1439.56
318.15	1.01201	1.0135 1.01360	–	–
323.15	1.00794	1.00956 1.0098	–	–
		p-cresol		
303.15	1.02620	1.02639 1.0263 1.0265	1470.24	1471.38 1471 1468.43
308.15	1.02230	1.02250 1.0225	–	–
313.15	1.01839	1.018593 1.0188	1439.5	1439.97 1439.56
318.15	1.01448	1.014661 1.0139	–	–
323.15	1.01055	1.010701 1.0102	–	–

Furthermore, Fig. 1 and Fig. 2 at 303.15K and 313.15K offered representations of the V^E data.

The following is the order in which 1,3-dichlorobenzene and isomeric cresols interact molecularly:

(1,3-dichlorobenzene + *o*-cresol) > (1,3-dichlorobenzene+*p*-cresol) > (1,3-dichlorobenzene +*m*-cresol)

The higher unfavorable surplus quantity within the entire system implies greater effectiveness in wrapping and/or dipole-dipole interactions between molecules while 1,3-dichlorobenzene and *o*-cresol were accompanied. In overall, the occurrence of undesirable aberrations form perfection in such binary liquid systems has been triggered by significant intermolecular interactions such as Interactions with dipoles and H bonds between various molecules are other intervening responses[31-33].

Excess isentropic compressibilities (κ_s^E)

Table 3, Table 4, Table 5, Table 6, Table 7 and Table 8 provided information for the binary combinations of 1,3 dichlorobenzene with *o*-, *m*-, and *p*-cresol at 303.15K and 313.15K, including the mole fraction (x_i), fictitious noise's the acceleration. (u), calculated noise acceleration, information from mathematical equations, isentropic the compressibility (KS), and surplus isentropic its compressibility (KSE) according to Redlich-Kister specifications.

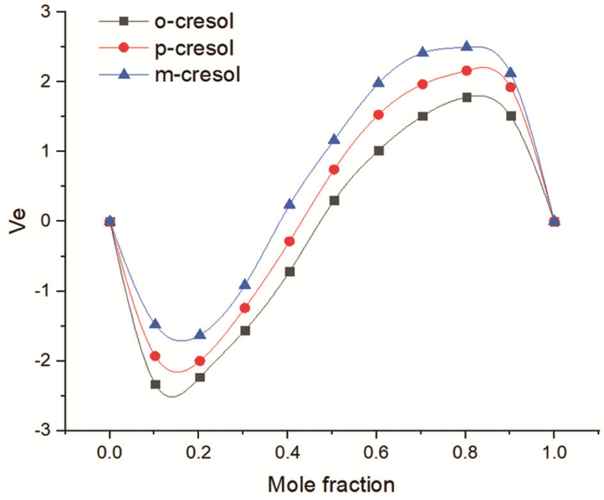

Fig. 1 — Variation of excess volume (V^E) of the binary liquid mixture of 1,3-dichlorobenzene (1) with *o*-cresol (2) (■), *m*-cresol (2) (●), *p*-cresol (2) (▼), at 303.15 K

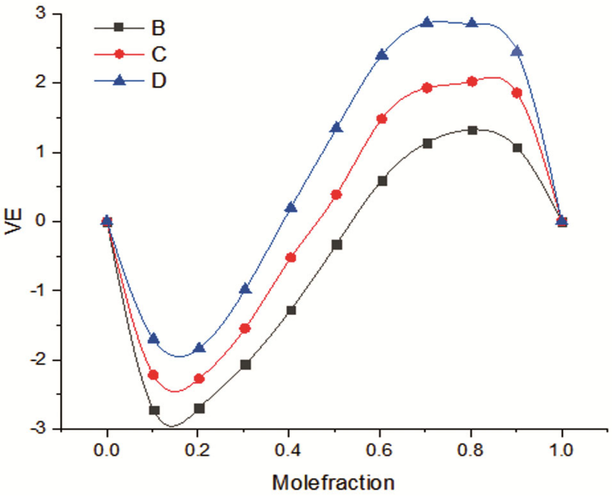

Fig. 2 — Variation of excess volume (V^E) of the binary liquid mixture of 1,3-dichlorobenzene (1) with *o*-cresol (2) (■), *m*-cresol (2) (●), *p*-cresol (2) (▼), at 313.15 K

Table 3 — 1,3-Dichlorobenzene (1)+*o*-cresol (2) at T=303.15 K

0	1.03651	0.000	0
0.102204	1.08805	–2.331	–2.330
0.202973	1.11362	–2.229	–2.228
0.303895	1.13257	–1.561	–1.562
0.404443	1.14901	–0.714	–0.715
0.50462	1.16323	0.300	0.301
0.604427	1.180169	1.018	1.019
0.703866	1.19919	1.511	1.512
0.80294	1.22041	1.785	1.784
0.901651	1.24755	1.513	1.513
1	1.28899	0.000	0

Table 4 — 1,3-Dichlorobenzene (1)+*o*-cresol (2) at T=313.15 K

0	1.0262	0.000	0
0.102204	1.083209	–2.717	–2.715
0.202973	1.11254	–2.694	–2.695
0.303895	1.13484	–2.065	–2.066
0.404443	1.15444	–1.275	–1.275
0.50462	1.17127	–0.333	–0.334
0.604427	1.18709	0.594	0.595
0.703866	1.205911	1.139	1.140
0.80294	1.227379	1.323	1.322
0.901651	1.25226	1.071	1.071
1	1.28482	0.000	0

Table 5 — 1,3-Dichlorobenzene (1) +*p*-cresol (2) at T=303.15

0	1.0262	0.000	0
0.102204	1.13337	–1.930	–1.931
0.202973	1.09358	–1.998	–1.997
0.303895	1.10995	–1.239	–1.240
0.404443	1.124293	–0.283	–0.283
0.50462	1.13792	0.746	0.745
0.604427	1.15458	1.530	1.531
0.703866	1.17578	1.966	1.966
0.80294	1.20057	2.161	2.160
0.901651	1.23194	1.923	1.923
1	1.28899	0.000	0

Table 6 — 1,3-Dichlorobenzene (1) +*p*-cresol (2) at T=313.15 K

0	1.01839	0.000	0
0.102203546	1.06377	–2.215	–2.215
0.203907848	1.08897	–2.278	–2.278
0.305116554	1.10621	–1.554	–1.555
0.405833278	1.12022	–0.523	–0.524
0.506061598	1.13578	0.385	0.386
0.605805059	1.14926	1.483	1.484
0.70506717	1.17088	1.923	1.924
0.803851408	1.19739	2.022	2.023
0.902161215	1.2284	1.850	1.851
1	1.28482	0.000	0

Table 7 — 1,3-Dichlorobenzene (1) + *m*-cresol (2) at T=303.15 K

0	1.02436	0.000	0
0.102690722	1.06239	–1.478	–1.479
0.204769248	1.08823	–1.628	–1.628
0.306241035	1.10522	–0.912	–0.913
0.407111476	1.11751	0.238	0.239
0.507385903	1.13238	1.167	1.166
0.60706958	1.14873	1.982	1.982
0.706167715	1.16994	2.415	2.416
0.80468545	1.19608	2.498	2.499
0.90262787	1.22913	2.126	2.130
1	1.28899	0.000	0

Table 8 — 1,3-Dichlorobenzene (1)+*m*-cresol (2) at T=313.15 K

0	1.01605	0.000	0
0.102690722	1.05634	–1.697	–1.670
0.204769248	1.0824	–1.833	–1.834
0.306241035	1.09842	–0.984	–0.984
0.407111476	1.1109	0.196	0.196
0.507385903	1.12378	1.344	1.344
0.60706958	1.13777	2.400	2.400
0.706167715	1.158927	2.865	2.870
0.80468545	1.18654	2.852	2.900
0.90262787	1.22033	2.444	2.446
1	1.28482	0.000	0

Furthermore, the KS^E values for each one of these binary fluid mixtures at 303.15 K and 313.15 K, correspondingly, were graphically shown in Fig. 1 and Fig. 2.

Calculating the isentropic compressibility (K^S) required using data on exploratory porosity (ρ) and the velocity of sound (u)[34].

$$\kappa_s = u^{-2}\rho^{-1} \qquad \ldots(2)$$

The appropriate surplus isentropic compressibility's (κsE) have been determined using the subsequent equation.

$$\kappa_s^E = \kappa_s - \kappa_s^{id} \qquad \ldots(3)$$

Along the optimum quantity of the isentropic compressibility, KS^{id}, was found utilizing the aforementioned formula. The KS^{id} had been given using the wording Benson and Kiyohara preferred[35].

$$\kappa_s^{id} = \sum_{i=1}^{2}\phi_i\left[\kappa_{s,i} + TV_i\left(\alpha_i^2\right)/C_{p,i}\right] - \left\{T\left(\sum_{i=1}^{2}x_iV_i\right)\left(\sum_{i=1}^{2}\phi_i\alpha_i\right)^2 \Big/ \sum_{i=1}^{2}x_iC_{p,i}\right\} \qquad \ldots(4)$$

Here, Cpi and αi represent the expansion of heat parameter as well as relative thermal capacity of the i^{th} ingredient, accordingly. Statistics for Cpi and αi were evaluated after obtaining them form the available information[36-38].

The free length theory (FLT) was used to examine the experimental sound speed. A comparison of theoretical and experimental sound speed readings indicates that the FLT model provides a more accurate estimate of sound speed data. Tables 3 to 8 also included the evaluating the scientifically large quantities (V^E) and κ_s^E quantities through utilizing the Redlich-Kister formula. It was explained how to calculate V^E using the Redlich-Kister equation[39,40].

The information that follows corresponds to the suggested scientific relationship by Redlich-Kister:

$$V^E/cm^3.mol^{-1} = X_1(1-X_1)[a_0 + a_1(2X_1-1) + a_2(2X_1-1)^2]$$

In the Redlich-Kister equation, a_0, a_1, a_2, while b_0, b_1, and b_2 are quantities that may be evolved, and X_i is the proportion of the equivalents containing aspects i (i = 1, 2) that constitute the altogether.

Conclusions

In this article that we present the experimental results for 1,3-dichlorobenzene's density and sound speed in binary mixtures which includes *o*-, *m*-, or *p*-cresol at temperatures within 303.15K, 323.15K; 303.15K and 313.15K, specifically. Redlich-Kister and formulation were utilized for evaluating the practical surplus capacity information as well as the recorded velocity of noise information in compared against the theoretical model (FLT). The interaction among 1,3-dichlorobenzene and *o*-cresol mixtures is more powerful than that involving 1,3-dichlorobenzene and *p*-cresol / *m*-cresol permutations.

Acknowledgements

The authors are thankful to the Department of Chemistry, Sri Venkateswara University in Tirupati, India, for letting them use their labs.

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