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Data Article

Excess volume, speed of sound and isentropic compressibility data of ternary mixtures containing N-methylcyclohexylamine, *p*-xylene and (C_3-C_5) 1-alkanols

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ABSTRACT

Excess volume (V^E_{123}) and speed of sound (u_{123}) data of three ternary mixtures of N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-alkanols (C_3-C_5) were determined as a function of composition at 303.15 K and atmospheric pressure. From the measured data, isentropic compressibility (k_{s123}), deviation in isentropic compressibility ($k_s{}'_{123}$) and the quantity $\Delta k_{s123,}$ the difference between measured value and that of computed from the constituent binary data were derived. The V^E_{123} data of all the mixtures were analyzed in terms of different theoretical models. The experimental and predicted results indicate that the theoretical expressions give good estimation of the derived functions for the studied ternary systems. The excess and deviation properties were discussed in terms of intermolecular interactions prevailing between component molecules in the liquid mixtures.

Specifications Table

Subject area	Physical Chemistry, Chemical Engineering, Chemical Thermodynamics
Compounds	N-methylcyclohexylamine, p-xylene and 1-alkanols
Data category	Physicochemical properties, Density, ultrasound velocity
Data acquisition format	Chemical data analysis
Data type	Calculated, analyzed
Procedure	Density measurements are made by using single-stem bicapillary pycnometer of bulb capacity 12 cm^3, and speeds of sound are estimated with single crystal ultrasonic interferometer (model F-82) from Mittal Enterprises, New Delhi, India
Data accessibility	Data is with this article

1. Rationale

Thermodynamic investigation of liquid mixtures is of great interest because of their extensive utilization in process designing, petrochemical industry, textile industry, pharmaceutical industry and in many other chemical engineering appli-

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cations. When two or more solvent molecules are associated with one another it results in significant differences in their intermolecular interactions. In recent years, measurement of excess volumes and isentropic compressibilities has been adequately employed in understanding molecular interactions in pure liquids and in liquid mixtures [1–4]. Keeping both the industrial and scientific interest in mind, many studies pertaining to thermophysical properties of binary mixtures have been reported in the literature, whereas the same for the ternary systems in particular are scarce. Hence in the present work, we report here new excess volume and deviation in isentropic compressibility data of ternary mixtures containing NMC and *p*-xylene with 1-alkanols (C_3-C_5) at T = 303.15 K and atmospheric pressure.

NMC has wide application in the production of pharmaceuticals, insecticides and pesticides [5]. Xylenes are used in printing, rubber and leather industries. Alkanols are extensively utilized in the manufacture of fuel, perfumes, cosmetics, paints, varnishes, drugs, explosives, fats, waxes, resins, etc., [6]. Because of their extensive industrial applications, knowledge of their thermophysical properties is of great importance from a practical point of view. Therefore, these systems have been selected in order to study the molecular interactions between NMC, *p*-xylene and 1-alkanols (C_3-C_5). In addition, the ternary V^E_{123} data of all the mixtures were analyzed in terms of predictive expressions [7–9]. The experimental data were discussed in terms of molecular interactions between component molecules.

2. Procedure

2.1. Reagents

All chemicals used were of analytical grade. N-methylcyclohexylamine (NMC) (>99.5% of purity) and 1-propanol (>99.7% of purity) were obtained from Sigma Aldrich. *m*-Xylene (>99.5% of purity), 1-butanol (>99.5% of purity) and 1-pentanol (>99.5% of purity) were purchased from Merck. All the chemicals were purified by the standard methods described in the literature [10–11]. The chemical names, acronyms, CAS numbers, molar mass, supplier, and molecular purities of the liquids used were reported in Table 1. The purities of the samples were checked by comparing the measured densities *(ρ)* and speed of sound *(u)* of the components with those reported in the literature [12-14] and these values were presented in Table 2.

2.2. Apparatus and procedures (Measurements)

A single-stem bicapillary pycnometer (made of borosil glass) of bulb capacity 12 cm^3 was utilized for density measurements. Excess volume (V^E_{123}) data for the ternary mixtures were measured using dilatometer [15]. The mixing cell contained three bulbs of different capacities that were connected by a W-tube. Mercury was used to separate three component liquids. One of the three bulbs was fitted with a capillary and the other two were fitted with ground-glass stoppers. Each bulb of the dilatometer was filled with a component whose mass was determined directly by weighing. The entire dilatometer was placed in a thermostat that could be maintained to 303.15 ± 0.01 K. All the measurements were made at constant temperature employing a thermostat. The measured ternary excess volume data (V^E_{123}) were accurate to ± 0.003 cm^3 mol^{-1}.

The speeds of sound data (u123) were measured [3] by a single crystal ultrasonic interferometer (model F-82) from Mittal Enterprises, New Delhi, India. A thermostatically controlled, well-stirred circulated water bath with a temperature controlled to ±0.01 K was used to maintain temperature stability. The uncertainty in sound speed measurement was is ± 0.3%.

Table 1
Characteristics of liquids used in the present work.

Material	Provenance	Molar mass ($g.mol^{-1}$)	CAS number	Mass fraction purity
N-methylcyclohexylamine (NMC)	Sigma-Aldrich, India.	113.2	100-60-7	99.5%
1-propanol	Sigma-Aldrich, India.	60.1	71-23-8	99.7%
1-butanol	Merck, India.	74.1	71-36-3	99.5%
1-pentanol	Merck, India.	88.1	71-41-0	99.5%

Table 2
Density (ρ) and speed of sound (u) of pure components at 303.15 K and atmospheric pressure.

Compound	ρ ($g.cm^{-3}$) Experimental	Literature	u ($m.s^{-1}$) Experimental	Literature
N-methyl cyclohexylamine	0.84683	0.84686 [12]	1356	1354 [12]
p-xylene	0.85229	0.85230 [13]	1289	1290 [13]
1-propanol	0.79566	0.79602 [14]	1189	1192 [14]
1-butanol	0.80205	0.80203 [14]	1229	1227 [14]
1-pentanol	0.80764	0.80764 [14]	1256	1258 [14]

Table 3
Mole fractions of N-methylcyclohexylamine (x_1), *p*-xylene (x_2), experimental and predicted excess volumes for the ternary mixtures of N-methylcyclohexylamine (NMC) (1) + p-xylene (2) + 1-alkanols (3) at 303.15 K and atmospheric pressure.

x_1	x_2	V^E (cm^3. mol^{-1}) Experimental	(Redlich-Kister)	Kohler	Tsao-Smith	Hwang	$\Delta V^E{}_{123}{}^*$
N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-propanol (3)							
0.1010	0.0741	-0.522	-0.525	-0.507	-0.537	-0.550	0.003
0.1113	0.1021	-0.564	-0.567	-0.546	-0.597	-0.595	0.003
0.2224	0.1341	-0.968	-0.974	-0.962	-1.056	-1.014	0.006
0.2092	0.2847	-0.720	-0.732	-0.739	-0.925	-0.801	0.012
0.1729	0.3429	-0.577	-0.590	-0.598	-0.798	-0.649	0.013
0.0564	0.4634	-0.197	-0.210	-0.201	-0.308	-0.229	0.013
0.1373	0.5423	-0.292	-0.306	-0.322	-0.517	-0.359	0.014
0.1658	0.6216	-0.223	-0.238	-0.248	-0.379	-0.301	0.015
0.1275	0.6712	-0.161	-0.172	-0.182	-0.322	-0.219	0.011
0.1626	0.7631	-0.110	-0.117	-0.100	-0.061	-0.166	0.007
0.1056	0.8323	-0.070	-0.074	-0.068	-0.052	-0.107	0.004
0.0801	0.8616	-0.049	-0.052	-0.049	-0.052	-0.078	0.003
N-methylcyclohexylamine (NMC) (1) + p-xylene (2) + 1-butanol (3)							
0.0800	0.049	-0.330	-0.331	-0.324	-0.332	-0.343	0.001
0.1034	0.1026	-0.407	-0.409	0.397	-0.434	-0.426	0.002
0.1204	0.159	-0.198	-0.202	-0.203	-0.384	-0.468	0.004
0.0807	0.2251	-0.284	-0.293	-0.283	-0.351	-0.310	0.009
0.0937	0.3429	-0.265	-0.277	-0.273	-0.377	-0.297	0.012
0.0992	0.4126	-0.236	-0.249	-0.249	-0.369	-0.271	0.013
0.1115	0.5012	-0.196	-0.211	-0.217	-0.354	-0.239	0.015
0.1124	0.5624	-0.156	-0.170	-0.177	-0.312	-0.198	0.014
0.0918	0.6209	-0.095	-0.106	-0.112	-0.232	-0.130	0.011
0.0823	0.6714	-0.062	-0.069	-0.073	-0.183	-0.090	0.007
0.1108	0.7326	-0.072	-0.077	-0.080	-0.154	-0.104	0.005
0.0878	0.8409	-0.041	-0.044	-0.044	-0.049	-0.067	0.003
N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-pentanol (3)							
0.0510	0.081	-0.265	-0.267	-0.270	-0.293	-0.246	0.002
0.1057	0.1534	-0.455	-0.457	-0.466	-0.539	-0.451	0.002
0.0930	0.201	-0.382	-0.385	-0.398	-0.483	-0.377	0.003
0.0648	0.2709	-0.25	-0.255	-0.269	-0.349	-0.247	0.005
0.0966	0.3392	-0.303	-0.309	-0.330	-0.455	-0.300	0.006
0.1081	0.4298	-0.264	-0.273	-0.296	-0.446	-0.267	0.009
0.0654	0.5436	-0.114	-0.126	-0.143	-0.265	-0.123	0.012
0.1818	0.6121	-0.197	-0.211	-0.223	-0.310	-0.228	0.014
0.0678	0.6762	-0.068	-0.079	-0.093	-0.214	-0.081	0.011
0.0992	0.7126	-0.094	-0.104	-0.117	-0.222	-0.112	0.010
0.0477	0.7562	-0.024	-0.032	-0.040	-0.137	-0.035	0.008
0.0676	0.8532	-0.044	-0.049	-0.053	-0.087	-0.062	0.005

$\Delta V^E{}_{123} = V^E{}_{123}(\text{Exp}) - V^E{}_{123}(\text{bc})$
Where $V^E{}_{123}(\text{bc})$ is computed from constituent binary data using Redlich-Kister equation.

3. Data, value and validation

3.1. Excess volume

The measured excess volume data ($V^E{}_{123}$) of three ternary liquid mixtures containing NMC and *p*-xylene with 1-propanol, 1-butanol and 1-pentanol at 303.15 K and atmospheric pressure were reported in Table 3 along with those values calculated from predictive expressions namely Redlich-Kister, Kohler, Tsao-Smith and Hwang et al. equations. These data were also graphically depicted in Figs. 1–3.

Redlich-Kister equation [7,8] can be expressed as:

$$V^E_{123} = \sum_{i<j} V^E_{ij}(x_i, x_j) \tag{1}$$

where $V^E_{ij} = x_i x_j \sum_{s=0}^{n} (A_s)_{ij}(x_i - x_j)^s$ and x_i, x_j are the mole fractions of the components in a ternary mixture.

Kohler Expression [7]:

$$V^E_{123} = (x_1 + x_2)^2 V^E_{12} + (x_1 + x_3)^2 V^E_{13} + (x_2 + x_3)^2 V^E_{23} \tag{2}$$

where $V^E_{ij} = x'_i x'_j \sum_{s=0}^{n} (A_s)_{ij}(x'_i - x'_j)^s$ at composition (x'_i, x'_j), such that $x'_i = 1 - x'_j = \frac{x_i}{x_i + x_j}$ where x_i and x_j are the ternary mole fractions.

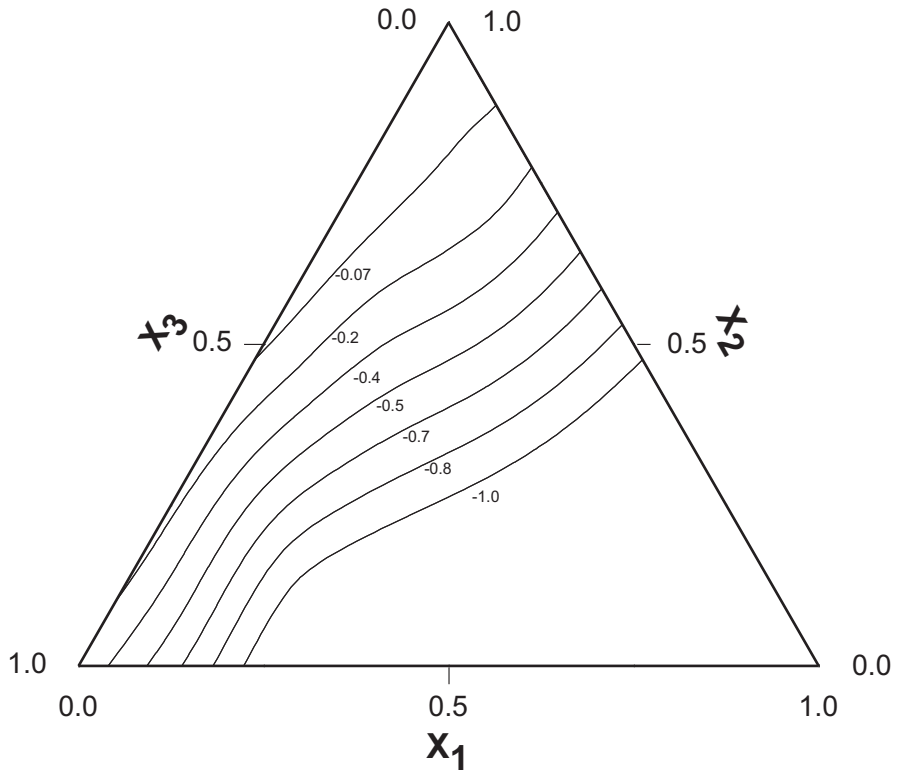

Fig. 1. Excess volumes (V^E_{123}) data for N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-propanol (3) at 303.15 K.

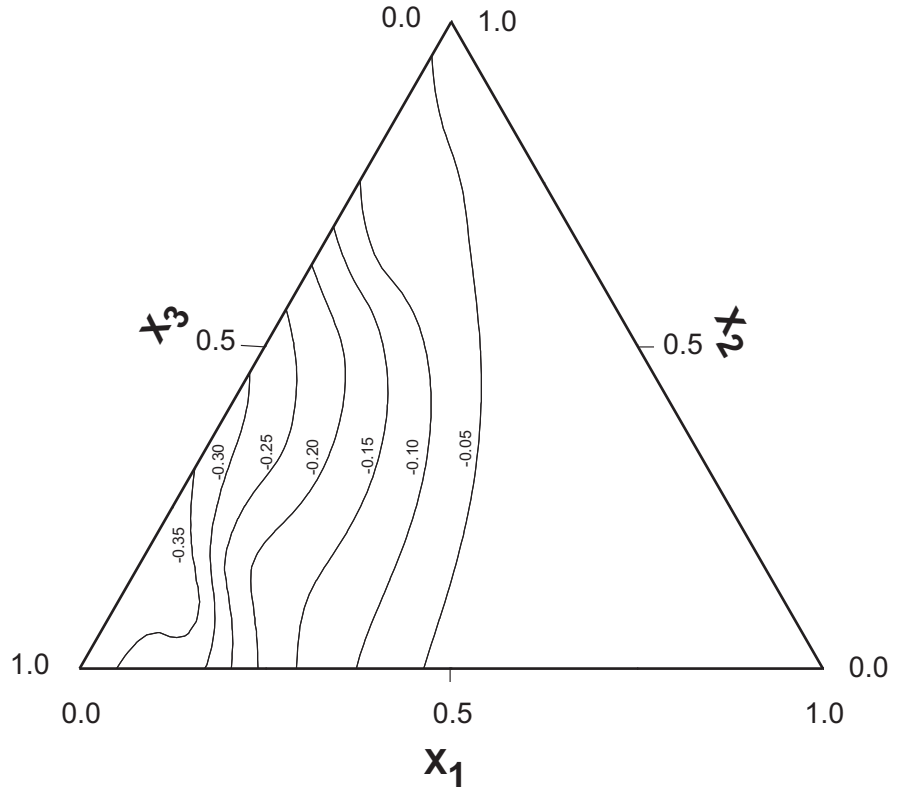

Fig. 2. Excess volumes (V^E_{123}) data for N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-butanol (3) at 303.15 K.

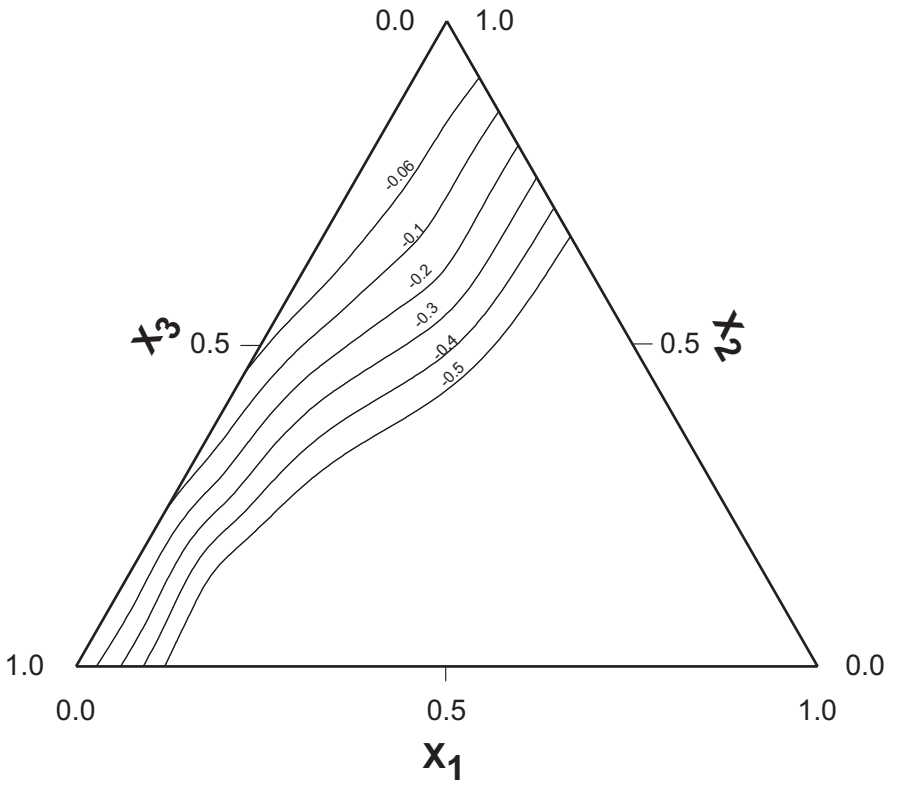

Fig. 3. Excess volumes (V^E_{123}) data for N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-pentanol (3) at 303.15 K.

Table 4
The standard deviation values (Redlich-Kister and Hwang eqns) of binary systems of $\sigma(V^E)$ at 303.15 K.

System	Redlich-Kister a_0	a_1	a_2	$\sigma(V^E)$	Hwang b_0	b_1	b_2	$\sigma(V^E)$
	cm^3mol^{-1}							
N-methyl cyclohexylamine (1)+ *p*-xylene (2)	-0.122	1.220	0.009	0.002	-0.125	1.464	-1.440	0.008
p-xylene (2)+ 1-propanol (3)	-0.076	0.560	0.463	0.000	-0.230	1.285	-0.050	0.006
p-xylene (2) + 1-butanol (3)	0.125	0.576	0.359	0.000	0.005	1.164	-0.207	0.000
p-xylene (2) + 1-pentanol (3)	0.090	0.371	0.027	0.002	0.081	0.477	-0.406	0.007
N-methyl cyclohexylamine (1) +1-propanol (3)	-6.237	2.703	3.925	0.002	-7.545	8.449	2.015	0.002
N-methyl cyclohexylamine (1) +1-butanol (3)	-5.219	0.847	1.908	0.001	-5.852	3.461	1.531	0.002
N-methyl cyclohexylamine (1) +1-pentanol (3)	-5.243	0.955	0.417	0.002	-5.382	1.695	-0.580	0.003

Tsao–Smith expression [7] is of the form:

$$V^E_{123} = x_2(1+x_1)^{-1}V^E_{12} + x_3(1-x_1)^{-1}V^E_{13} + (1-x_1)V^E_{23} \tag{3}$$

where V^E_{12}, V^E_{13} and V^E_{23} are the binary excess volumes at composition (x'_i, x'_j), such that $x'_i = x_1$ for 1,2 and 1,3 binary systems and $x'_2 = \frac{x_2}{x_2+x_3}$ for 2,3 binary system.

Hwang et al. equation [9]:

$$V^{E(123)}/cm^3mol^{-1} = x_1x_2\left(b_0^{(12)} + b_1^{(12)}x_1^3 + \ +b_2{}^{(12)}x_2{}^3\right) + x_1x_3\left(b_0^{(13)} + b_1^{(13)}x_1^3 + \ +b_3^{(13)}x_3^3\right)$$
$$+x_2x_3\left(b_0^{(23)} + b_2^{(23)}x_2^3 + \ +b_3^{(23)}x_3^3\right) \tag{4}$$

The quantity $\Delta V^E{}_{123}$, difference between measured ternary data and computed from the constituent binary data through the Redlich-Kister relation were given in last column of Table 3. The binary data which was used to compute ternary excess volume data for the mixtures NMC+*m*-xylene [12], NMC+1-alkanols [16] and *p*-xylene +1-alkanols [17] were collected from the literature and these data were included in Table 4 along with standard deviation values $\sigma(V^E)$.

The sign and magnitude of $V^E{}_{123}$ data depends upon the resultant of the following factors [18]:

i dissociation of associated alkanols in solution systems

ii donor-acceptor interaction between π-electrons of the aromatic ring and the alkanols
iii a possible inclusion of *p*-xylene into the structural network of alkanols.

The first factor contributes to expansion in volume and the second and third factors lead to contraction in volume. The experimental V^E_{123} data in Table 2 suggest that the combined effects for volume contraction i.e., donor-acceptor interactions and inclusion of *p*-xylene into the structural network of alkanols exceed the factors responsible for volume expansion.

The molecular interaction between NMC and 1-alkanols in the studied ternary mixtures can be explained as follows [19]. Negative contributions in the mixtures containing NMC and 1-alkanol arise from two factors: a) changes in free volumes in the real mixtures and b) the presence of electron donor-acceptor interactions between NMC and 1-alkanol. The negative V^E_{123} values in the present ternary system emphasis that the breaking of the three-dimensional associated network of the alkanol is incomplete and that the aromatic hydrocarbon molecules are more or less fitted into the alkanol networks.

In addition, specific interactions due to the formation of N––H•••π type hydrogen bond between NMC and electrons in aromatic ring of *p*-xylene also contribute significantly to negative V^E_{123} data of the studied ternary mixtures [12].

A perusal of Table 3 clearly indicates that V^E_{123} data is more negative for the ternary mixtures containing 1-propanol and the negative value decreases with increase in chain length from 1-propanol to 1-pentanol. The effect of increasing chain length of 1-alkanol on the V^E_{123} data can be considered using the effective dipole moment. The negative V^E_{123} values decrease with decreasing effective dipole moment of 1-alkanol in the systems of cyclic amine with alcohols [6] which can be explained as follows. The dipole moment of 1-alkanols decreases with increase in chain length. Polarity of hydroxyl group also decreases with increase in chain length of 1-alkanol. These two factors result in the rupture of alkanol-alkanol hydrogen bonds. Moreover, in higher alkanols, hydroxyl group proton will be shielded by the adjacent methyl groups, thus availability of such protons will be diminished for the formation heteroassociates which ultimately results in decrease in negative V^E_{123} data in higher 1-alkanols [4] in the following order:1-propanol > 1-butanol >1-pentanol.

An examination of ternary data in Table 3 reveal that the predictive expressions proposed by Redlich-Kister, Kohler, Tsao-Smith and Hwang et al. gives satisfactory estimation in terms of ternary excess volumes in all the mixtures.

3.2. Isentropic compressibility

The isentropic compressibility of ternary mixtures (κ_{s123}) was calculated from the expression

$$\kappa_{s123} = u^{-2}{}_{123}\rho^{-1}{}_{mix123} \tag{5}$$

where u_{123} and $\rho_{\mathrm{mix}123}$ indicate speed of sound and density of ternary mixtures respectively.

The density of a ternary liquid mixture (ρ_{mix123}) was computed using the expression

$$\rho_{mix123} = x_1M_1 + x_2M_2 + x_3M_3/V + V^E{}_{123} \tag{6}$$

where x_1, x_2 and x_3 represent mole fractions and M_1, M_2 and M_3 are the molecular weights of NMC, *p*-xylene and 1-alkanols respectively; V is the molar volume of the mixture and V^E_{123} is ternary excess volume.

The deviation in isentropic compressibility (κ'_{s123}) was estimated using the relation

$$\kappa'_{s123} = k_{s123} - \text{ø}_1k_{s1} - \text{ø}_2k_{s2} - \text{ø}_3k_{s3} \tag{7}$$

where ø_1, ø_2, ø_3, κ_{s1}, κ_{s2} and κ_{s3} are the volume fractions and isentropic compressibilities of the pure components 1, 2 and 3 respectively. The quantity $\Delta\kappa_{s123}$, the difference between measured value of $\kappa_s{}'_{123}$ and that of computed from binary data $\kappa'_{s123\,(b)}$ has been calculated using the relation

$$\Delta\kappa_{s\,123} = \kappa'_{s\,123} - \kappa'_{s\,123\,(b)} \tag{8}$$

The latter quantity, $\kappa_s{}'_{123(b)}$ was computed using Redlich-Kister relation [8]

$$\kappa'_{s123\,(b)} = \kappa_{s12} + \kappa_{s13} + \kappa_{s23} \tag{9}$$

where κ_{s12}, κ_{s13} and κ_{s23} denote the deviation in isentropic compressibilities for the three binary mixtures and these are estimated using the smoothing equation

$$\kappa_{sij} = \text{ø}_1\text{ø}_2\left[a_0 + a_1(\text{ø}_1 - \text{ø}_2) + a_2(\text{ø}_1 - \text{ø}_2)^2\right] \tag{10}$$

where a_0, a_1 and a_2 are the constants obtained by the method of least squares. Further, the binary parameters that were required to compute $k_s{}'_{123(b)}$ for the mixtures of NMC with *p*-xylene [20], NMC with 1-alkanols [21] and *p*-xylene with 1-alkanols [17] were collected from the literature and these were given in Table 5 along with standard deviation $\sigma(\Delta\kappa_s)$.

The speed of sound (u), density of the mixture (ρ_{mix123}), isentropic compressibility (κ_{s123}), deviation in isentropic compressibility (κ'_{s123}) and the quantity $\Delta\kappa_{s123}$, the difference between measured data of $\kappa_s{}'_{123}$ and that of computed from the constituent binary data $\kappa'_{s123\,(b)}$ were presented in Table 6. Moreover, the deviation in isentropic compressibility ($\Delta\kappa_{s123}$) for the three ternary mixtures was also graphically represented in Figs. 4–6.

An examination of $\Delta\kappa_{s123}$ values in Table 6 suggest that the values were positive over the entire composition range in all the binary mixtures of NMC and *p*-xyleme with 1-alkanols and these were 3 to 4 times to the experimental error.

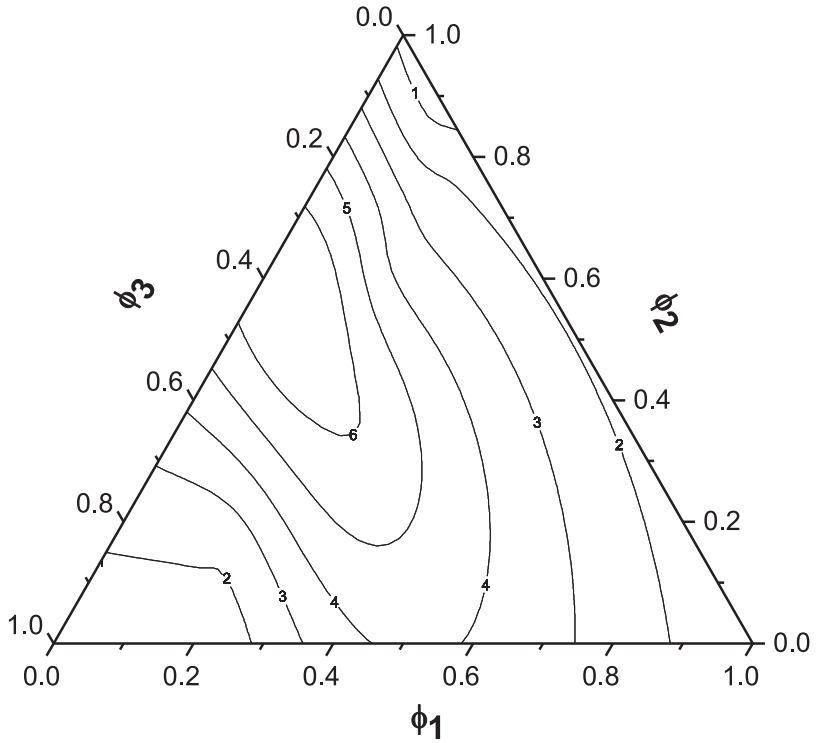

Fig. 4. Deviation in isentropic compressibility ($\Delta\kappa_{s123}$) data for N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-propanol (3) at 303.15 K.

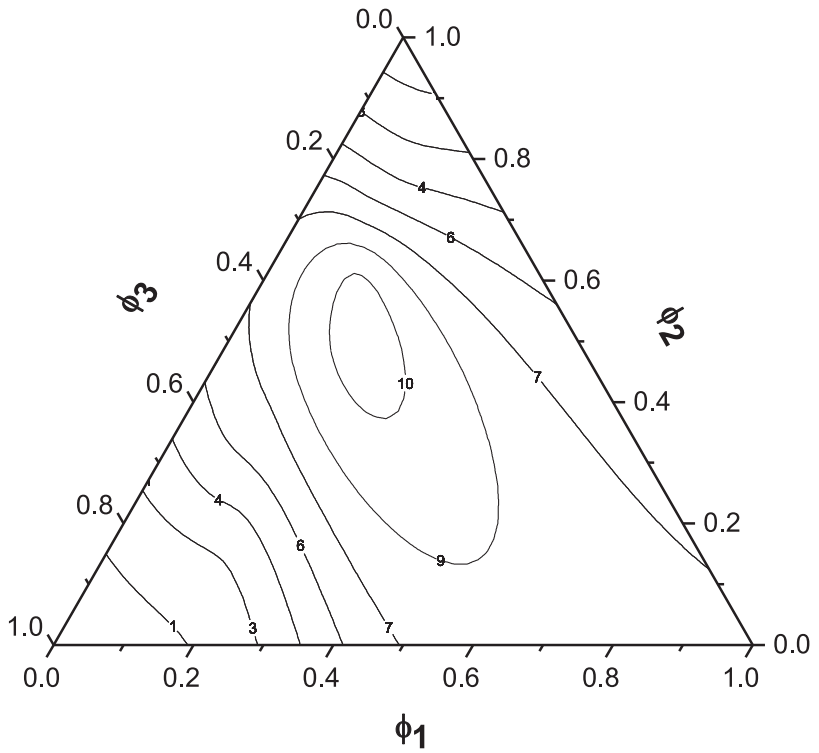

Fig. 5. Deviation in isentropic compressibility ($\Delta\kappa_{s123}$) data for N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-butanol (3) at 303.15 K.

Table 5
The standard deviation $\sigma(k_s)$ values of all the binary systems computed from Redlich-Kister equation at 303.15 K.

System	a_0 TPa-1	a_1	a_2	$\sigma(k_s)$
N-methyl cyclohexylamine (1)+ *p*-xylene (2)	-21.80	33.60	24.01	2
p-xylene (2)+1-propanol (3)	35.13	106.01	40.15	2
p-xylene (2)+ 1-butanol (3)	62.49	112.94	7.07	0
p-xylene (2)+ 1-pentanol (3)	80.95	138.16	32.51	0
N-methyl cyclohexylamine (1)+1-propanol (3)	-219.00	35.40	-68.30	2
N-methyl cyclohexylamine (1)+1-butanol (3)	-166.50	21.84	89.70	2
N-methyl cyclohexylamine (1)+1-pentanol (3)	-147.50	3.05	61.40	3

Table 6
Volume fractions of N-methylcyclohexylamine (ϕ_1), p-xylene (ϕ_2), density (ρ), speed of sound (u_{123}), isentropic compressibility (k_{s123}), deviation in isentropic compressibility (κ_{s123}), deviation in isentropic compressibility computed from constituent binary data $(\kappa_{s123(b)})$ and $\Delta\kappa_{s123}$ values for ternary systems N-methylcyclohexylamine (NMC) (1) + p-xylene (2) +1-alkanols (3).

Φ1	Φ2	P (g.cm^3)	U (m.s^{-1})	κ_{s123}	κ_{s123} TPa-1	$\kappa_{s123(b)}$	$\Delta\kappa_{s123}$
N-methylcyclohexylamine (NMC) (1) p-xylene (2) + 1-propanol (3)							
0.1587	0.1085	0.81490	1238	800	-29	-31	2
0.1709	0.1461	0.81796	1244	790	-29	-31	2
0.1127	0.7157	0.83005	1254	766	-33	-37	4
0.275	0.3488	0.83539	1271	741	-16	-22	6
0.2257	0.4171	0.83551	1267	745	-11	-17	6
0.0742	0.5685	0.83323	1248	771	6	-1	7
0.1667	0.6135	0.84110	1274	732	-2	-6	4
0.1916	0.6695	0.84498	1286	715	-3	-6	3
0.1471	0.7216	0.84520	1283	719	0	-3	3
0.1775	0.7766	0.84946	1298	699	-2	-4	2
0.1152	0.8466	0.84995	1295	702	-1	-2	1
0.0874	0.8766	0.85008	1292	705	0	-1	1
N-methylcyclohexylamine (NMC) (1) + p-xylene (2) + 1-butanol (3)							
0.1099	0.0629	0.81287	1250	787	-12	-13	1
0.1382	0.1278	0.81799	1258	772	-14	-16	2
0.157	0.1932	0.82036	1265	762	-12	-15	3
0.1047	0.2723	0.82267	1255	772	-2	-7	5
0.1167	0.3961	0.82930	1257	763	7	0	7
0.1208	0.4682	0.83275	1258	759	12	3	9
0.1317	0.5519	0.83710	1261	751	16	6	10
0.1305	0.6085	0.83958	1263	747	19	8	11
0.1056	0.6658	0.84089	1264	744	19	11	8
0.0937	0.7124	0.84245	1266	740	18	12	6
0.1229	0.7571	0.84606	1279	722	11	7	4
0.0953	0.8511	0.84933	1288	710	6	4	2
N-methylcyclohexylamine (NMC) (1) + p-xylene (2) + 1-pentanol (3)							
0.0611	0.0904	0.81599	1269	761	-5	-6	1
0.1238	0.1675	0.82324	1277	745	-7	-10	3
0.1086	0.2187	0.82439	1273	748	-2	-6	4
0.0754	0.2937	0.82548	1269	752	4	0	4
0.1106	0.362	0.83027	1271	746	8	2	6
0.122	0.4522	0.83374	1270	744	14	7	7
0.0734	0.5685	0.83667	1263	749	22	18	4
0.1975	0.6197	0.84438	1286	716	10	7	3
0.0747	0.6948	0.84204	1266	740	23	20	3
0.1082	0.7243	0.84484	1275	728	18	15	3
0.0523	0.7723	0.84430	1268	737	23	21	2
0.0729	0.8574	0.84905	1283	715	11	10	1

This suggests that Redlich-Kister equation is capable of giving good estimation of deviation in isentropic compressibility of ternary mixtures from that of constituent binaries [17,20,21].

The deviation in isentropic compressibility $(\Delta\kappa_{s123})$ data in the studied ternary mixtures is influenced by three factors: i) structure-breaking effects ii) structure making effects and iii) change in geometrical factors [2]. Structure breaking effects contribute to an increase in free spaces [22] between the molecules leading to positive deviation in compressibility. On the other hand, structure making effect and geometrical effect cause decrease in free spaces of the component molecules on mixing there by leading to negative deviation in isentropic compressibility. The actual deviation would depend up on

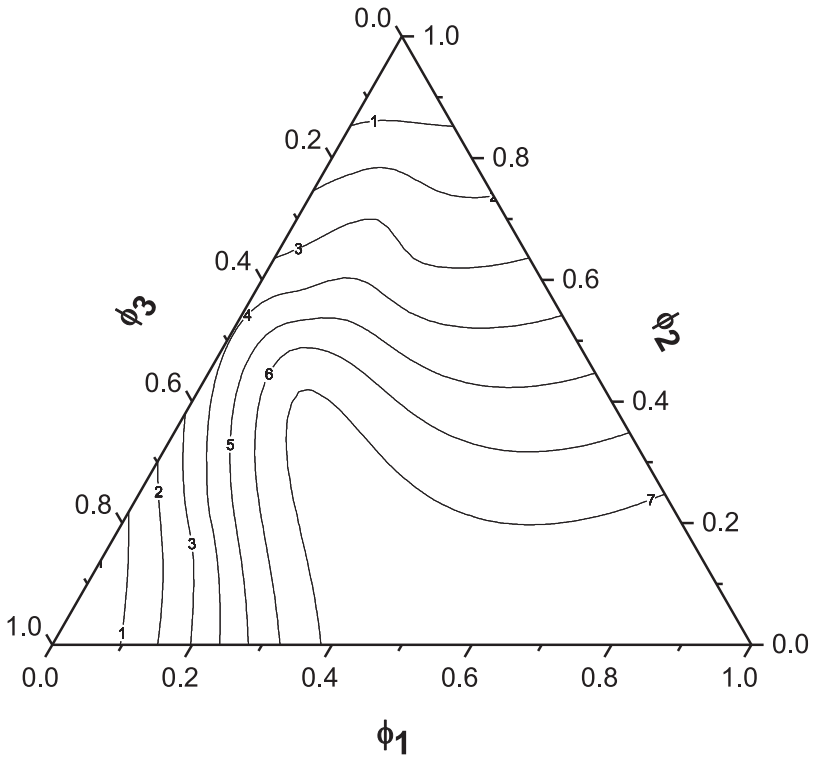

Fig. 6. Deviation in isentropic compressibility ($\Delta\kappa_{s123}$) data for N-methylcyclohexylamine (NMC) (1) + *p*-xylene (2) + 1-Pentanol (3) at 303.15 K.

Table 7
The standard deviation values $\sigma(\Delta V^E_{123})$ and $\sigma(\Delta\kappa_{s123})$ for ternary systems of N- methylcyclohexylamine (NMC) (1) + p-xylene (2)+1-alkanols (3).

system	A	B	C		A	B	C	
	$cm^3\ mol^{-1}$			$\sigma(\Delta V^E_{123})$	TPa^{-1}			$\sigma(\Delta\kappa_{s13})$
NMC (1) + *p*-xylene (2)+ 1-propanol(3)	0.639	2.026	-11.054	0.003	243.51	609.37	-4292.23	3
NMC (1) + *p*-xylene (2) + 1-butanol(3)	0.617	-11.177	-92.757	0.005	389.68	1843.89	-13821.03	1
NMC (1) + *p*-xylene (2) + 1-pentanol(3)	691.209	-1.737	-64.668	0.006	298.12	29.10	-20220.44	0

the balance between these two opposing effects. The experimental $\Delta\kappa_{s123}$ values indicate that structure breaking effect is dominant in all the three ternary mixtures.

The experimental ΔV^E_{123} and $\Delta\kappa_{s123}$ data were fitted to the following equation proposed by Redlich-Kister [8]:

$$\Delta V^E_{123}/cm^3mol^{-1} = x_1x_2x_3\left[A + Bx_1(x_2 - x_3) + C\,x_1^2(x_2 - x_3)^2\right] \tag{11}$$

$$\Delta\kappa_{s123}/TPa^{-1} = \phi_1\phi_2\phi_3\left[A + B\,\phi_1(\phi_2 - \phi_3) + C\,\phi_1^2(\phi_2 - \phi_3)^2\right] \tag{12}$$

where *A*, *B* and *C* are the ternary constants which were calculated by least square method. The values of coefficients were inturn used to compute standard deviation $\sigma(Y^E_{123})$.

$$\sigma\left(Y^E_{123}\right) = \left[\Sigma\left(Y^E_{123\ exp} - Y^E_{123\ cal}\right)^2/(m-n)\right]^{1/2} \tag{13}$$

where $\sigma(Y^E_{123}) = \Delta V^E_{123}$ (or) Δk_{s123}

'*m*' is the total number of experimental points and '*n*' is the number of coefficients in Equation (11) and (12) and the values of ternary constants A, B and C along with their standard deviation values were given in Table 7.

4. Conclusions

In the present investigation, excess volume, sound speed and deviation in isentropic compressibility data were reported for three ternary mixtures of N-methylcyclohexylamine (NMC) + *p*-xylene + 1-propanol or + 1-butanol + 1-pentanol at

303.15 K and atmospheric pressure. Experimental excess volume data were found to be negative as a function of composition. The negative V^E_{123} data for the studied systems follow the order: 1-propanol > 1-butanol >1-pentanol. Whereas (Δk_{s123}) data were found to be positive for all the ternary mixtures. The experimental ternary (V^E_{123}) data were compared with theoretical models proposed by Redlich-Kister, Kohler, Tsao-Smith and Hwang et al. and found in good agreement between the predicted and experimental data. The V^E_{123} $\Delta\kappa_{s123}$ parameters were analyzed interms of intermolecular interactions between component molecules.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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