Thermodynamic and topological investigations of mixtures containing lactams with cyclic ketones: Excess molar volumes and excess isentropic compressibilities

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Abstract: The densities, ρ_{123} and speeds of sound, u_{123} data of ternary N-methylpyrrolidin-2-one (1) + pyrrolidin-2-one (2) + cyclopentanone or cyclohexanone (3) mixtures have been measured over entire mole fraction at 293.15, 298.15, 303.15 and 308.15 K. The experimental densities and speeds of sound data have been utilized to evaluate excess molar volumes, V^{E}_{123} and excess isentropic compressibility, $\left(\kappa^{E}_{S}\right)_{123}$ of the studied ternary mixtures. The results indicate that V^{E}_{123} and $\left(\kappa^{E}_{S}\right)_{123}$ of N-methylpyrrolidin-2-one (1) + pyrrolidin-2-one (2) + cyclopentanone or cyclohexanone (3) mixtures are negative over entire composition range. The V^{E}_{123} and $\left(\kappa^{E}_{S}\right)_{123}$ data have been analyzed in terms of Graph theory. It has been observed that Graph theory correctly predicts the sign and magnitude of the excess molar volumes and excess isentropic compressibilities of the studied ternary mixtures.

Keywords
Excess molar volumes, Excess isentropic compressibilities, Connectivity parameter of third degree of a molecule, $^{3}\xi$, interaction parameter, χ

1. Introduction

The experimental data on thermodynamic properties of liquid mixtures are of considerable interest for selecting appropriate liquid mixtures in different applications of chemical engineering and industries [1-2]. These properties are required for their use in the design and operation of chemical reactions, pumps and heat transfer equipment. Proper design and development of separation processes are conditioned by an adequate knowledge on thermodynamic properties of liquids used in the processes. N-methylpyrrolidin-2-one is non-aqueous, thermally stable, nontoxic and is a preferred selective crystallization solvent [3]. Pyrrolidin-2-one is a cyclic amide (lactam) and on the basis of ab initio studies [4], an enveloped confirmation is assigned to pyrrolidin-2-one. Further, pyrrolidin-2-one or its derivatives have shown significant biological and pharmacological activities [5-6]. In these applications, mixtures of lactams with organic liquids can be preferred, if the mixed solvent functions effectively [7]. Cyclic alkanones are versatile solvents that are used in the synthesis of pharmaceuticals, in agricultural chemistry and as flavoring agents [8-9].Mixtures composed of N-methylpyrrolidin-2-one, pyrrolidin-2-one with Cycpentanone or cyclohexanone thus comprise a substantial portion of liquid mixtures of practical importance in industries. In continuation of our earlier studies on thermodynamic properties like excess molar volumes, V^{E} and excess isentropic compressibilities, κ^{E}_{S} data of N-methylpyrrolidin-2-one (1) + pyrrolidin-2-one (2) and N-methylpyrrolidin-2-one or pyrrolidin-2-one (1) + cyclopentanone or cyclohexanone (2) binary mixtures[10-11], we report here densities, ρ and speeds of sound, u of N-methylpyrrolidin-2-one (1) + pyrrolidin-2-one (2) + cyclopentanone or cyclohexanone (3) mixtures at 293.15, 298.15, 303.15 and 308.15 K. An attempt has been made to determine V^{E}_{123} and $\left(\kappa^{E}_{S}\right)_{123}$ of ternary mixtures using Graph theory.

Experimental

N-methylpyrrolidin-2-one (NMP) (Fluka, 0.99 GC), pyrrolidin-2-one (2-Py) (Fluka, 0.99 GC), cyclopentanone (CPO)(Fluka, 0.99 GC) and cyclohexanone(CHO) (Fluka, 0.99 GC), were purified by standard methods [12-14]. The densities and speeds of sound values of the purified liquids are presented and compared with literature values [15-26] in Table 1.

Densities, ρ and speeds of sound, u values of the pure liquids and their ternary mixtures were measured using a commercial density and sound analyzer apparatus (Anton Paar DSA-5000) in the manner as described elsewhere [27-28].

The apparatus was calibrated with double distilled deionised water. The mole fraction of each mixture was obtained with standard uncertainty of 1 x 10^{-4} from the measured apparent masses of the components. All the measurements were performed on an electric balance Mettler AX-205 Delta Range with an uncertainty of $\pm 10^{-5}$ g. The density and speed of sound can be measured to $\pm$ 10^{-3} kg·m^{-3} and 10^{-2} m·s^{-1}, respectively. The standard uncertainties in the density and speed of sound measurements are 0.5 kg·m^{-3} and 0.1 m·s^{-1} respectively. Further, the standard uncertainty in V^E values predicted from density results is 0.1 %.

2. Results

The experimental densities, ρ_{123}; speeds of sound, , u_{123} of NMP (1) + 2-py (2) + CPO or CHO (3) mixtures were measured at 293.15 to 308.15 K at atmospheric pressure are summarized in Table 2. The excess molar volumes, V_{123}^{E} and excess isentropic compressibilities, $\left(\kappa_{\mathrm{S}}^{\mathrm{E}}\right)_{123}$ for the investigated ternary mixtures were calculated using

$$V_{123}^{\mathrm{E}}=\sum_{\mathrm{i}=1}^{3} x_i M_i(\rho_{ijk})^{-1}-\sum_{\mathrm{i}=1}^{3} x_i M_i(\rho_i)^{-1} \tag{1}$$

$$(\kappa_{\mathrm{S}})_{123}=\left(\rho_{123}u_{123}^2\right)^{-1} \tag{2}$$

$$(\kappa_{\mathrm{S}}^{\mathrm{E}})_{123}=(\kappa_{\mathrm{S}})_{123}-\kappa_{\mathrm{S}}^{\mathrm{id}} \tag{3}$$

where x_i, M_i, ρ_i (i = 1 or 2 or 3) are the mole fraction, molar mass and densities of component i. The, ρ_{123}; u_{123}; $(\kappa_{\mathrm{S}})_{123}$ are the densities, speeds of sound and isentropic compressibilities of ternary mixtures respectively. The ideal contribution $\kappa_{\mathrm{S}}^{\mathrm{id}}$ for (1+2+3) mixtures were estimated by Benson and Kiyohara [29] equation

$$\kappa_{\mathrm{S}}^{\mathrm{id}}=\sum_{\mathrm{i}=1}^{2\mathrm{or}3}\phi_{\mathrm{i}}\left[\kappa_{\mathrm{S,i}}+\frac{Tv_{\mathrm{i}}\alpha_{\mathrm{i}}^2}{C_{\mathrm{p,i}}}\right]-T\left(\sum_{\mathrm{i}=1}^{2\mathrm{or}3}x_{\mathrm{i}}v_{\mathrm{i}}\right)\frac{\left(\sum_{\mathrm{i}=1}^{2\mathrm{or}3}\phi_{\mathrm{i}}\alpha_{\mathrm{i}}\right)^2}{\left(\sum_{\mathrm{i}=1}^{2\mathrm{or}3}x_{\mathrm{i}}C_{\mathrm{p,i}}\right)} \tag{4}$$

where ϕ_i, $\kappa_{\mathrm{S,i}}$, v_{i}, α_{i} and $C_{\mathrm{p,i}}$ (i = 1 or 2 or 3) are volume fraction, isentropic compressibility, molar volume, thermal expansion coefficient and molar heat capacity of pure component (i), T is the temperature. The α values for the liquids were obtained using experimental densities values in the manner as suggested elsewhere [30]. The C_{p} values of NMP, 2-py and CPO or CHO were taken from literature [10-11]. The V_{123}^{E} and, $\left(\kappa_{\mathrm{S}}^{\mathrm{E}}\right)_{123}$ data for the present mixtures are listed in Tables 3 respectively.

The results of V_{123}^{E} and $\left(\kappa_{\mathrm{S}}^{\mathrm{E}}\right)_{123}$ were fitted to Redlick-Kister equation to show their dependence on composition using

$$Y_{123}^{\mathrm{E}}(X=V\mathrm{or}\ \kappa_{\mathrm{S}})=x_1x_2\left[\sum_{\mathrm{n}=0}^{2}(Y_{12}^{(\mathrm{n})})(x_1-x_2)^{\mathrm{n}}\right]+x_2x_3\left[\sum_{\mathrm{n}=0}^{2}(Y_{23}^{(\mathrm{n})})(x_2-x_3)^{\mathrm{n}}\right]$$
$$+x_1x_3\left[\sum_{\mathrm{n}=0}^{2}(Y_{13}^{(\mathrm{n})})(x_1-x_3)^{\mathrm{n}}\right]+x_1x_2x_3\left[\sum_{\mathrm{n}=0}^{2}(Y_{123}^{(\mathrm{n})})(x_2-x_3)^{\mathrm{n}}x_1^{\mathrm{n}}\right] \tag{5}$$

The $Y_{123}^{(\mathrm{n})}$ (n = 0-2) are characteristic parameters of (1+2+3) ternary mixtures respectively. These parameters were obtained by fitting measured results to Eq. (5) using least square regression method. The resulting parameters along with standard deviations, expressed by relations:

$$\sigma(Y_{123}^{\mathrm{E}})=\{[\sum Y_{123}^{\mathrm{E}}-Y_{123\ \{\mathrm{calc.\ Eq.\ (5)}\}}^{\mathrm{E}}]^2/(\mathrm{m}-\mathrm{n})\}^{0.5} \tag{6}$$

{where m is the number of data points and n is the number of adjustable parameters of Eq. (5)} are recorded in Table 3. Further, various surfaces generated by V_{123}^{E} and $\left(\kappa_{\mathrm{S}}^{\mathrm{E}}\right)_{123}$ values [28] {evaluated by employing equation (5)} for the investigated mixtures are shown in Figs. 1-2 & 3-4 respectively. The V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ values in Figs. 1- 4 were obtained (corresponding to 1-2 axis) by keeping x_3 constant and varying the values of x_1 and x_2 (shown as red line); V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ values (corresponding to 1-3 axis) were obtained by keeping x_2 constant and varying the values x_1 and x_3 (shown as green line).

3. Discussion

The V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ data of the studied ternary mixtures are not reported in literature with which present data be compared. The V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ of NMP (1) + 2-py (2) + CPO or CHO (3) mixtures are negative over entire composition range. The V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ data of the present (1+2+3) mixtures provides information about the molecular arrangement and molecular interactions operating among the constituent mixtures. The negative V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ values suggests a more packed arrangement of NMP or 2-py or CPO or CHO in their mixed state as compared to pure state and also attractive molecular interactions among the constituents of mixtures. The V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ values for NMP (1) + 2-py (2) + CHO (3) mixtures are more negative than those of NMP (1) + 2-py (2) + CPO (3) mixtures. It may be due to reason that contribution to V^{E}_{123} and $(\kappa^{E}_{S})_{123}$ due to rupturing of associated NMP:CHO molecular entity is more than that of NMP:CPO. The $\partial V^{E}_{123}/\partial T$ and $\partial(\kappa^{E}_{S})_{123}/\partial T$ for the studied mixtures are positive.

4. Graph theory

Excess molar volumes and excess isentropic compressibilties of ternary mixtures

The analysis of V^{E}_{12} and $(\kappa^{E}_{S})_{12}$ data of NMP or 2-py (1) + CPO or CHO (2) has indicated that NMP and 2-py exist as associated molecular entity while CPO or CHO exist as a mixture of cyclic and open dimer[10,11]. The NMP (1) + 2-py (2) + CPO or CHO (3) ternary mixtures formation may then be assumed to be comprised of processes (1) establishment of unlike (a) 1_n- 2_n (b) 2_n - 3_n (c) 1_n- 3_n contacts; (2) unlike contact formation weakens 1-1, 2-2 and 3-3 interactions and leads to their depolymerisation; and (3) monomers of 1, 2 and 3 then undergo interactions to form (a) 1:2 (b) 2:3 and (c) 1:3 molecular complexes. If χ_{12}, χ_{23}, χ_{13} and χ'_{11}, χ'_{22}, χ'_{33} are the molar volumes and molar compressibilities interaction parameters for unlike contacts 1_n- 2_n, 2_n - 3_n, 1_n- 3_n, contacts and depolymerisation of 1_n, 2_n, 3_n constituent molecules, then change in thermodynamic properties, ΔX ($X = V$ or κ_S) due to processes 1 (a) to (c) and (2) (a)-(b) were expressed [14-20] by

$$\Delta X_1 \ (X = V \text{ or } \kappa_S) = \left[\frac{x_1 x_2 \left({}^3\xi_1 / {}^3\xi_2\right)}{x_1 + x_2\left({}^3\xi_1 / {}^3\xi_2\right)}\right]\left[\chi_{12} + x_1 \chi'_{11}\right] \tag{14}$$

$$\Delta X_2 \ (X = V \text{ or } \kappa_S) = \left[\frac{x_2 x_3 \left({}^3\xi_2 / {}^3\xi_3\right)}{x_2 + x_3\left({}^3\xi_2 / {}^3\xi_3\right)}\right]\left[\chi_{23} + x_2 \chi'_{22}\right] \tag{15}$$

$$\Delta X_3 \ (X = V \text{ or } \kappa_S) = \left[\frac{x_3 x_1 \left({}^3\xi_3 / {}^3\xi_1\right)}{x_3 + x_1\left({}^3\xi_3 / {}^3\xi_1\right)}\right]\left[\chi_{13} + x_3 \chi'_{33}\right] \tag{16}$$

Further, if χ_{12}, χ'_{12}, χ''_{12} are interactions parameters for the formation of 1:2; 2:3 and 1:3 molecular complexes, then change in thermodynamic properties, ΔX ($X = V$ or κ_S) due to processes (3) (a)-(c) is given by

$$\Delta X_4 \ (X = V \text{ or } \kappa_S) = \left[\frac{x_1 x_2^2\left({}^3\xi_1 / {}^3\xi_2\right)}{x_1 + x_2\left({}^3\xi_1 / {}^3\xi_2\right)}\right]\left[\chi_{12}\right] \quad (17)$$

$$\Delta X_5 \ (X = V \text{ or } \kappa_S) = \left[\frac{x_2 x_3^2\left({}^3\xi_2 / {}^3\xi_3\right)}{x_2 + x_3\left({}^3\xi_2 / {}^3\xi_3\right)}\right]\left[\chi_{12}^{/}\right] \quad (18)$$

$$\Delta X_6 \ (X = V \text{ or } \kappa_S) = \left[\frac{x_3 x_1^2\left({}^3\xi_3 / {}^3\xi_1\right)}{x_3 + x_1\left({}^3\xi_3 / {}^3\xi_1\right)}\right]\left[\chi_{12}^{//}\right] \quad (19)$$

The total change in thermodynamic properties, $X_{123}^{E}(X = V \text{or } \kappa_S)$ due to processes 1 (a) to (c), (2) (a)-(b) and (3) (a)-(c) were then expressed by relation:

$$X_{ijk}^{E} \ (\mathrm{X} = V \text{ or } \kappa_S) = \left[\frac{x_1 x_2\left({}^3\xi_1 / {}^3\xi_2\right)}{x_1 + x_2\left({}^3\xi_1 / {}^3\xi_2\right)}\right]\left[\chi_{11} + x_1\chi_{11}^{/} + x_2\chi_{12}\right] + \left[\frac{x_2 x_3\left({}^3\xi_2 / {}^3\xi_3\right)}{x_2 + x_3\left({}^3\xi_2 / {}^3\xi_3\right)}\right]\left[\chi_{23} + x_2\chi_{22}^{/} + x_3\chi_{12}^{/}\right] + \left[\frac{x_3 x_1\left({}^3\xi_3 / {}^3\xi_1\right)}{x_3 + x_1\left({}^3\xi_3 / {}^3\xi_1\right)}\right]\left[\chi_{13} + x_3\chi_{33}^{/} + x_1\chi_{12}^{//}\right] \quad (20)$$

For the present mixtures, it was assumed that $\chi_{12} \cong \chi_{12} = \chi_{12}^{*}$; $\chi_{23} \cong \chi_{12}^{/} = \chi_{23}^{*}$; $\chi_{13} \cong \chi_{12}^{//} = \chi_{13}^{*}$; $\chi_{11}^{/} \cong \chi_{22}^{/} \cong \chi_{33}^{/} = \chi^{*}$, equation (20) was then reduced to

$$X_{123}^{E}(X = V \text{ or } \kappa_S) = \left[\frac{x_1 x_2\left({}^3\xi_1 / {}^3\xi_2\right)}{x_i + x_j\left({}^3\xi_i / {}^3\xi_j\right)}\right]\left[(1 + x_2)\chi_{12}^{*} + x_1\chi^{*}\right] + \left[\frac{x_2 x_3\left({}^3\xi_2 / {}^3\xi_3\right)}{x_2 + x_3\left({}^3\xi_2 / {}^3\xi_3\right)}\right]\left[(1 + x_3)\ \chi_{23}^{*} + x_2\chi^{*}\right] + \left[\frac{x_3 x_1\left({}^3\xi_3 / {}^3\xi_1\right)}{x_3 + x_1\left({}^3\xi_3 / {}^3\xi_1\right)}\right]\left[(1 + x_1)\chi_{13}^{*} + x_3\chi^{*}\right] \quad (21)$$

equation (21) contain four unknown χ_{12}^{*} etc. parameters and were evaluated by utilizing V_{123}^{E} and $\left(\kappa_S^E\right)_{123}$ data of (1 + 2 + 3) mixtures at four compositions. The resulting parameters were then used to determine X_{123}^{E} ($X = V$ or κ_S) data of the ternary mixture at other values of x_i and x_j . Such X_{123}^{E} ($X = V$ or κ_S) for the investigated mixtures are recorded in Table 4. The deviation between experimental and values of V_{123}^{E} , $\left(\kappa_S^E\right)_{123}$ predicted by Graph theory along with χ_{12}^{*} etc. parameters are recorded in Table 3. Examination of data in Table 4 has revealed that V_{123}^{E} and $\left(\kappa_S^E\right)_{123}$ values determined by Graph theory are in agreement with experimental values.

Conclusion:

Excess molar volumes and excess isentropic compresibities for ternary mixtures have been predicted from the measured densities and speeds of sound results at 293.15 to 308.15 at an interval of 5 K. Excess properties have been fitted to Redlich-Kister equation to find binary and ternary adjustable parameters and standard deviations. The comparison between experimental and calculated V_{123}^{E} and $\left(\kappa_S^{\mathrm{E}}\right)_{123}$ values (calculated from Graph theory) support various assumptions regarding the various processes involved in the present ternary mixtures.

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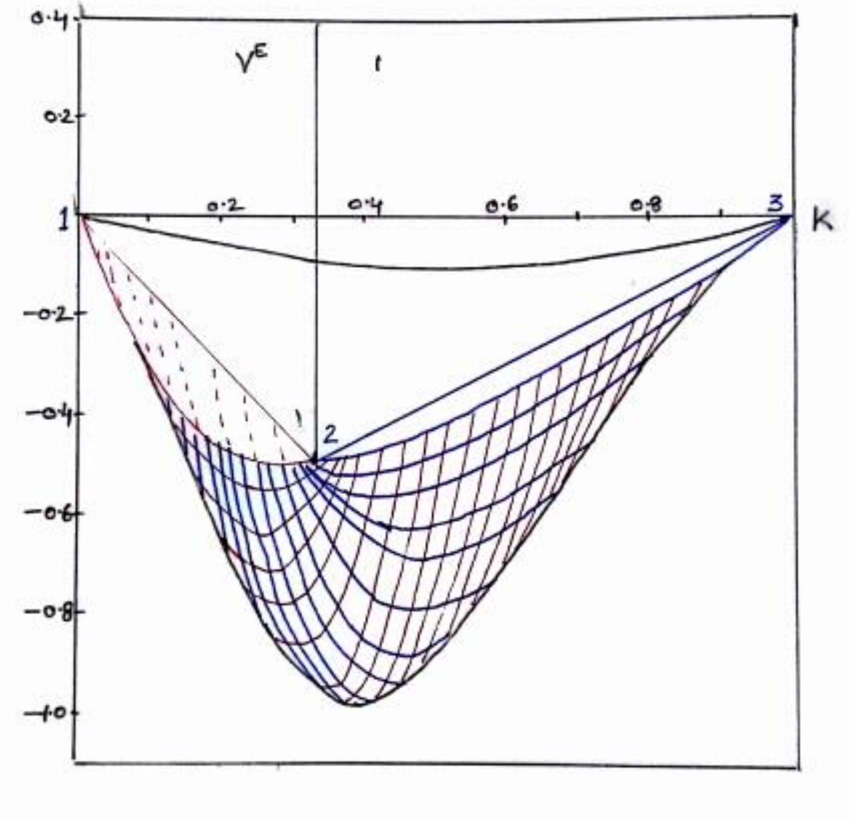

Fig-1

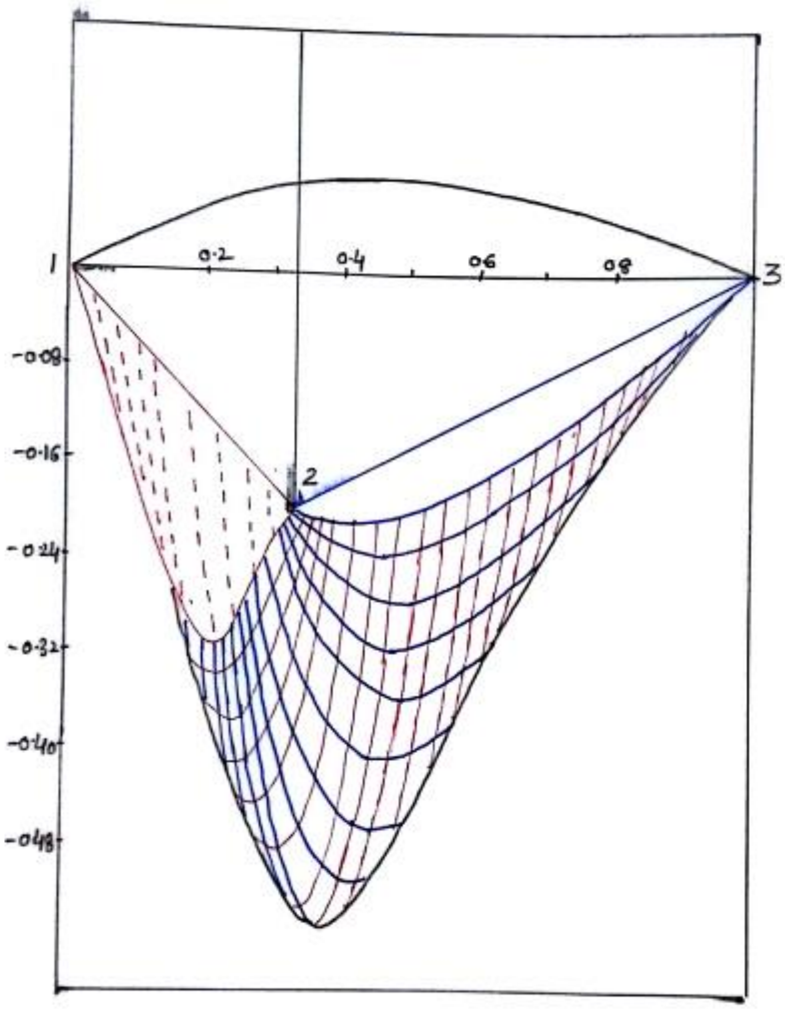

Fig-2

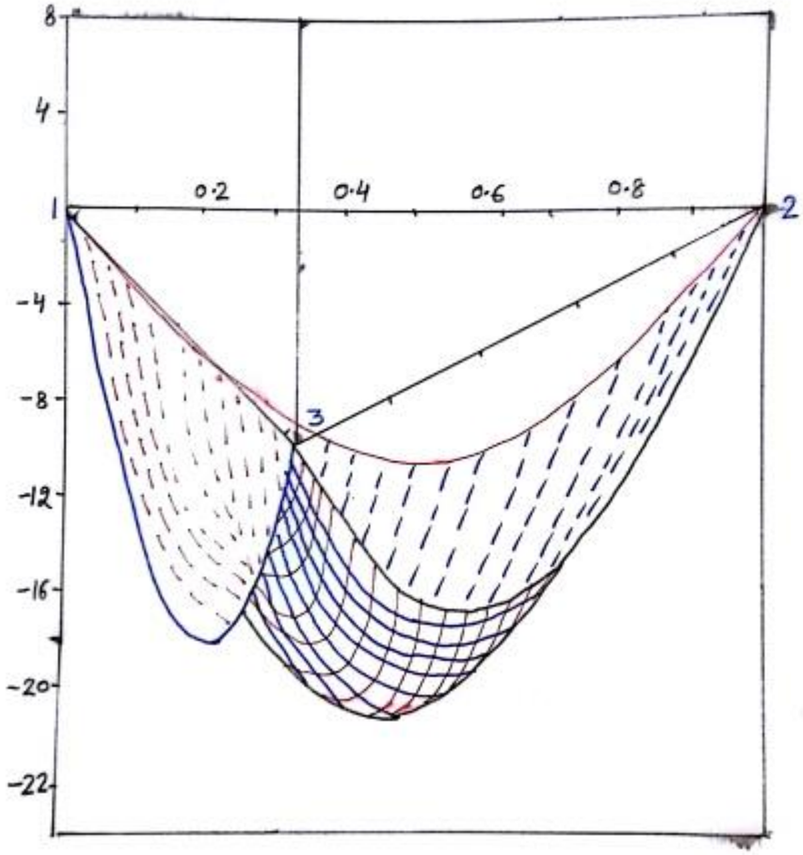

Fig-3

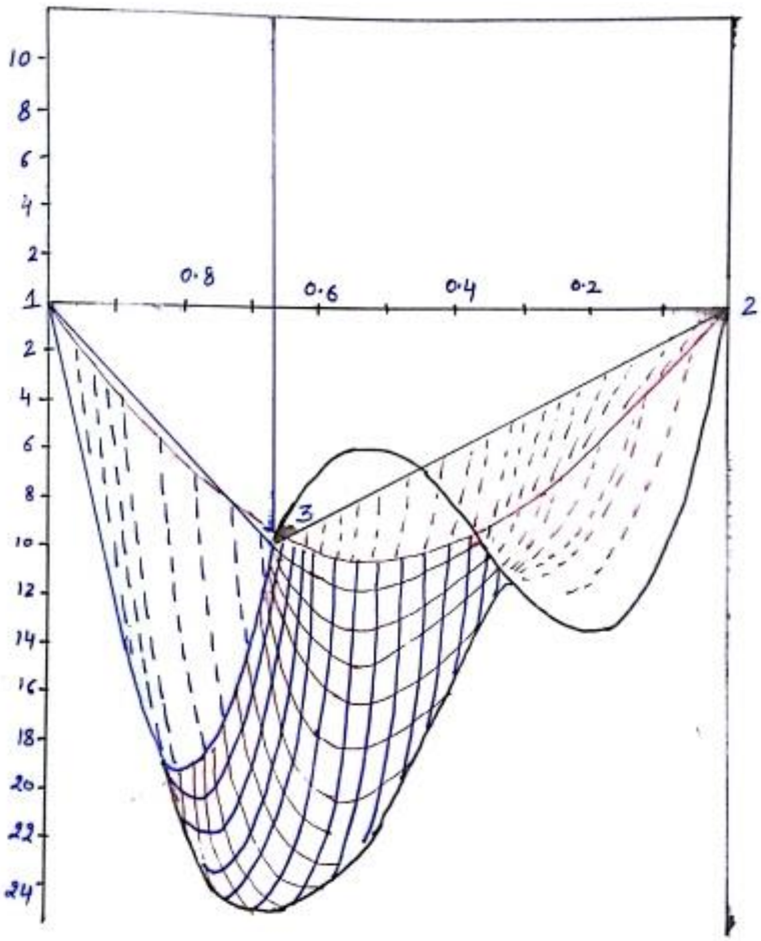

Fig-4

Figure Captions

Fig. 1 Excess molar volumes, V_{123}^{E} for N-methylpyrrolin-2-one (1) + pyrrolidin-2-one (2) + Cyclopentanone (3) ternary mixture at 298.15 K, the experimental data in front of the plane ( ); the experimental data behind the plane (---------).

Fig. 2 Excess molar volumes, V_{123}^{E} for N-methylpyrrolin-2-one (1) + pyrrolidin-2-one (2) + Cyclohexanone (3) ternary mixture at 298.15 K, the experimental data in front of the plane ( ); the experimental data behind the plane (---------).

Fig. 3 Excess isentropic compressibilities, $\left(\kappa_{S}^{E}\right)_{123}$ for N-methylpyrrolin-2-one (1) + pyrrolidin-2-one (2) + Cyclopentanone (3) ternary mixture at 298.15 K, the experimental data in front of the plane ( ); the experimental data behind the plane (---------).

Fig. 4 Excess isentropic compressibilities, $\left(\kappa_{S}^{E}\right)_{123}$ for N-methylpyrrolin-2-one (1) + pyrrolidin-2-one (2) + Cyclohexanone (3) ternary mixture at 298.15 K, the experimental data in front of the plane ( ); the experimental data behind the plane (---------).

Table 1 Comparison of densities, ρ, speeds of sound, u, with their literature values at T = (293.15, 298.15, 303.15, 308.15) K

Liquids	T/K	ρ (kg·m^{-3})		u (m·s^{-1})	
		Expt.	Lit.	Expt.	Lit.
N-Methyl pyrrolidin-2-one	293.15	1033.28	1033.23[15]	1565.59	1565.52[15]
	298.15	1028.26	1028.23[15]	1546.09	1546.02[15]
	303.15	1023.49	1023.46[15]	1527.31	1527.24[15]

	308.15	1018.69	1018.66[15]	1507.49	1507.38[15]
pyrrolidin-2-one	293.15	1111.28	1111.28[15]	1651.44	1650.13[15]
	298.15	1107.15	1107.15[15]	1635.02	1633.92[15]
	303.15	1103.06	1103.02[15]	1618.70	1617.14[15]
	308.15	1111.28	1111.28[15]	1651.44	1650.13[15]
Cyclopentanone	293.15	949.342	-	1414.25	-
	298.15	944.515	944.35 [16] 945.3 [17, 18]	1393.21	1394.1 [19]
	303.15	939.680	-	1372.50	-
	308.15	934.836	-	1352.57	-
Cyclohexanone	293.15	947.387	946.44 [20] 947.80 [21]	1431.89	1430.5 [26]
	298.15	942.904	942.76 [8] 942.4 [22]	1414.75	1408.0 [25] 1417.00 [22]
	303.15	938.051	937.4 [23] 940.3 [24]	1395.60	-
	308.15	933.181	933.8 [8] 935.7 [27] 936.5 [23]	1375.84	-

Table 2 Measured densities, ρ_{123}; excess molar volumes, V^{E}_{123}; speeds of sound, u_{123}; isentropic compressibilities, $(\kappa_S)_{123}$ and excess isentropic compressibilities, $(\kappa^{E}_{S})_{123}$ data compared with Graph theory for the various (1 + 2 + 3) mixtures as a function of mole fraction, x_1, of component (1) and x_2, of component (2) at T = (293.15, 298.15, 303.15 and 308.15) K

x_1	x_2	ρ_{123} (kg·m^{-3})	u_{123} / m·s^{-1}	V^{E}_{123} Expt. (cm^3·mol^{-1})	V^{E}_{123} (Graph) (cm^3·mol^{-1})	$(\kappa^{E}_{S})_{123}$ (Expt) (TPa^{-1})	$(\kappa^{E}_{S})_{123}$ (Graph) (TPa^{-1})	$(\kappa_S)_{123}$ (TPa^{-1})
0.1037	0.2725	1001.2	1492.1	-0.270	-0.267	-10.9	-10.5	448.7
0.1395	0.2680	1004.3	1497.4	-0.321	-0.319	-11.6	-11.5	444.1
0.1662	0.2578	1005.4	1499.8	-0.346	-0.346	-12.0	-12.0	442.2
0.1836	0.2530	1006.4	1501.8	-0.360	-0.361	-12.2	-12.3	440.6
0.2042	0.2485	1007.7	1504.4	-0.375	-0.377	-12.5	-12.6	438.5
0.2396	0.2389	1009.6	1508.3	-0.393	-0.396	-12.8	-13.0	435.4
0.2503	0.5674	1064.2	1594.8	-0.531	-0.592	-12.7	-13.0	369.4
0.2703	0.5432	1062.3	1592.6	-0.559	-0.604	-13.1	-13.4	371.1
0.2846	0.5194	1060.0	1589.2	-0.584	-0.608	-13.5	-13.7	373.5
0.3046	0.4884	1057.0	1585.0	-0.612	-0.609	-13.9	-14.0	376.6
0.3300	0.4534	1053.8	1580.7	-0.635	-0.607	-14.3	-14.2	379.8
0.3557	0.2048	1014.7	1520.3	-0.401	-0.408	-13.2	-13.4	426.4
0.3568	0.4530	1055.9	1586.1	-0.624	-0.624	-14.1	-14.1	376.4
0.3868	0.4139	1052.4	1581.3	-0.637	-0.612	-14.3	-14.2	380.0
0.3983	0.1941	1016.7	1525.0	-0.397	-0.401	-13.1	-13.3	423.0
0.4170	0.3987	1052.4	1583.0	-0.624	-0.614	-14.1	-14.1	379.2
0.4299	0.1773	1016.6	1526.1	-0.370	-0.383	-12.8	-12.9	422.4
0.4366	0.3460	1045.8	1572.1	-0.628	-0.571	-14.2	-14.1	386.9
0.4534	0.1755	1018.3	1529.6	-0.374	-0.379	-12.7	-12.8	419.7
0.4750	0.3456	1048.6	1579.2	-0.598	-0.583	-13.7	-13.7	382.4
0.4938	0.1591	1019.0	1532.1	-0.346	-0.354	-12.3	-12.3	418.1
0.5266	0.1490	1020.1	1534.9	-0.330	-0.336	-11.9	-11.9	416.1
0.5497	0.1468	1021.7	1538.0	-0.329	-0.329	-11.6	-11.6	413.8
0.5801	0.1367	1022.5	1540.2	-0.309	-0.309	-11.1	-11.1	412.2
0.6129	0.1220	1022.7	1541.6	-0.278	-0.280	-10.5	-10.4	411.5
0.6341	0.1200	1024.1	1544.3	-0.274	-0.273	-10.1	-10.1	409.4
0.6531	0.1122	1024.4	1545.2	-0.256	-0.256	-9.7	-9.7	408.9
0.6734	0.1062	1025.0	1546.7	-0.242	-0.242	-9.2	-9.3	407.8

0.6934	0.0993	1025.5	1547.9	-0.225	-0.226	-8.8	-8.8	407.0
0.7124	0.0937	1026.0	1549.3	-0.211	-0.213	-8.3	-8.4	406.1
0.1037	0.2725	997.4	1473.3	-0.337	-0.329	-12.7	-12.4	461.9
0.1395	0.2680	1000.7	1478.7	-0.404	-0.399	-13.5	-13.4	457.0
0.1662	0.2578	1001.9	1481.1	-0.438	-0.438	-13.9	-13.9	455.0
0.1836	0.2530	1002.9	1483.1	-0.457	-0.459	-14.2	-14.2	453.3
0.2042	0.2485	1004.3	1485.7	-0.478	-0.481	-14.5	-14.6	451.1
0.2396	0.2389	1006.2	1489.7	-0.503	-0.509	-14.8	-15.0	447.9
0.2503	0.5674	1060.7	1576.9	-0.607	-0.672	-13.8	-14.2	379.2
0.2703	0.5432	1058.8	1574.6	-0.640	-0.687	-14.3	-14.5	380.9
0.2846	0.5194	1056.5	1571.2	-0.671	-0.694	-14.8	-14.9	383.4
0.3046	0.4884	1053.5	1566.9	-0.705	-0.699	-15.3	-15.3	386.6
0.3300	0.4534	1050.4	1562.5	-0.735	-0.701	-15.7	-15.6	389.9
0.3557	0.2048	1011.3	1501.6	-0.520	-0.530	-15.1	-15.3	438.5
0.3568	0.4530	1052.4	1567.8	-0.717	-0.717	-15.4	-15.4	386.6
0.3868	0.4139	1048.9	1563.0	-0.736	-0.709	-15.7	-15.6	390.3
0.3983	0.1941	1013.2	1506.3	-0.514	-0.520	-15.0	-15.1	435.0
0.4170	0.3987	1048.8	1564.6	-0.719	-0.712	-15.4	-15.3	389.5
0.4299	0.1773	1013.0	1507.4	-0.482	-0.499	-14.6	-14.7	434.5
0.4366	0.3460	1042.3	1553.7	-0.736	-0.672	-15.7	-15.5	397.4
0.4534	0.1755	1014.8	1510.9	-0.485	-0.491	-14.5	-14.6	431.7
0.4750	0.3456	1045.0	1560.7	-0.693	-0.685	-15.0	-14.9	392.9
0.4938	0.1591	1015.3	1513.4	-0.449	-0.460	-14.0	-14.0	430.0
0.5266	0.1490	1016.3	1516.1	-0.427	-0.435	-13.5	-13.5	428.1
0.5497	0.1468	1017.9	1519.3	-0.423	-0.423	-13.2	-13.2	425.6
0.5801	0.1367	1018.6	1521.5	-0.397	-0.396	-12.6	-12.6	424.1
0.6129	0.1220	1018.7	1522.8	-0.356	-0.359	-11.9	-11.9	423.3
0.6341	0.1200	1020.1	1525.6	-0.349	-0.347	-11.5	-11.5	421.2
0.6531	0.1122	1020.2	1526.5	-0.326	-0.326	-11.0	-11.0	420.7
0.6734	0.1062	1020.8	1528.0	-0.307	-0.307	-10.5	-10.5	419.6
0.6934	0.0993	1021.2	1529.1	-0.285	-0.286	-10.0	-10.0	418.8
0.7124	0.0937	1021.7	1530.5	-0.266	-0.268	-9.4	-9.5	417.8
0.1037	0.2725	993.5	1454.0	-0.412	-0.401	-14.2	-14.1	476.1
0.1395	0.2680	997.0	1459.4	-0.498	-0.491	-15.1	-15.1	470.9
0.1662	0.2578	998.3	1461.8	-0.541	-0.541	-15.6	-15.6	468.8
0.1836	0.2530	999.4	1463.7	-0.567	-0.569	-15.9	-15.9	467.0
0.2042	0.2485	1000.8	1466.3	-0.594	-0.598	-16.2	-16.2	464.7
0.2396	0.2389	1002.8	1470.3	-0.627	-0.634	-16.5	-16.6	461.3
0.2503	0.5674	1057.0	1558.1	-0.678	-0.744	-14.7	-15.1	389.7
0.2703	0.5432	1055.1	1555.7	-0.714	-0.761	-15.2	-15.5	391.6
0.2846	0.5194	1052.9	1552.2	-0.751	-0.773	-15.7	-15.9	394.2
0.3046	0.4884	1050.0	1547.9	-0.794	-0.783	-16.3	-16.3	397.5
0.3300	0.4534	1046.9	1543.5	-0.833	-0.790	-16.8	-16.7	400.9
0.3557	0.2048	1008.0	1482.1	-0.651	-0.665	-16.7	-16.8	451.6
0.3568	0.4530	1048.8	1548.7	-0.802	-0.802	-16.4	-16.4	397.5
0.3868	0.4139	1045.4	1543.9	-0.831	-0.801	-16.7	-16.6	401.3
0.3983	0.1941	1009.9	1486.8	-0.644	-0.651	-16.5	-16.5	447.9
0.4170	0.3987	1045.2	1545.5	-0.808	-0.805	-16.4	-16.3	400.6
0.4299	0.1773	1009.6	1487.9	-0.605	-0.628	-16.0	-16.1	447.4
0.4366	0.3460	1039.0	1534.7	-0.849	-0.773	-17.0	-16.6	408.6
0.4534	0.1755	1011.4	1491.4	-0.607	-0.616	-15.9	-16.0	444.5
0.4750	0.3456	1041.4	1541.7	-0.786	-0.784	-16.1	-15.8	404.0
0.4938	0.1591	1011.8	1493.9	-0.563	-0.578	-15.3	-15.3	442.8
0.5266	0.1490	1012.7	1496.8	-0.534	-0.546	-14.8	-14.8	440.8
0.5497	0.1468	1014.2	1500.0	-0.528	-0.528	-14.4	-14.4	438.2
0.5801	0.1367	1014.9	1502.3	-0.494	-0.493	-13.8	-13.8	436.6
0.6129	0.1220	1014.9	1503.7	-0.443	-0.448	-13.0	-13.0	435.8
0.6341	0.1200	1016.2	1506.5	-0.432	-0.430	-12.6	-12.6	433.6
0.6531	0.1122	1016.3	1507.4	-0.403	-0.403	-12.1	-12.1	433.0
0.6734	0.1062	1016.8	1509.0	-0.379	-0.379	-11.5	-11.5	431.9
0.6934	0.0993	1017.1	1510.2	-0.351	-0.352	-10.9	-11.0	431.1
0.7124	0.0937	1017.6	1511.6	-0.328	-0.329	-10.4	-10.4	430.1
0.1037	0.2725	989.5	1435.4	-0.475	-0.455	-15.7	-15.9	490.5
0.1395	0.2680	993.0	1440.9	-0.572	-0.563	-16.7	-16.8	485.0

0.1662	0.2578	994.4	1443.2	-0.624	-0.624	-17.2	-17.2	482.8
0.1836	0.2530	995.5	1445.2	-0.654	-0.658	-17.5	-17.5	480.9
0.2042	0.2485	997.0	1447.8	-0.686	-0.692	-17.9	-17.8	478.5
0.2396	0.2389	999.0	1451.7	-0.725	-0.737	-18.2	-18.2	475.0
0.2503	0.5674	1053.0	1540.8	-0.732	-0.792	-15.9	-16.4	400.0
0.2703	0.5432	1051.1	1538.4	-0.770	-0.811	-16.4	-16.8	402.0
0.2846	0.5194	1048.8	1534.8	-0.810	-0.826	-17.0	-17.2	404.7
0.3046	0.4884	1046.0	1530.5	-0.857	-0.841	-17.6	-17.7	408.2
0.3300	0.4534	1042.9	1526.0	-0.900	-0.853	-18.2	-18.1	411.8
0.3557	0.2048	1004.2	1463.4	-0.759	-0.777	-18.3	-18.3	465.0
0.3568	0.4530	1044.6	1531.1	-0.862	-0.862	-17.7	-17.7	408.3
0.3868	0.4139	1041.2	1526.3	-0.896	-0.867	-18.1	-17.9	412.3
0.3983	0.1941	1006.1	1468.0	-0.751	-0.761	-18.1	-18.1	461.2
0.4170	0.3987	1041.0	1527.8	-0.869	-0.872	-17.8	-17.5	411.6
0.4299	0.1773	1005.7	1469.0	-0.708	-0.737	-17.6	-17.6	460.8
0.4366	0.3460	1034.9	1517.0	-0.926	-0.848	-18.6	-17.9	419.9
0.4534	0.1755	1007.4	1472.6	-0.709	-0.720	-17.4	-17.5	457.8
0.4750	0.3456	1037.1	1523.9	-0.850	-0.858	-17.5	-17.0	415.2
0.4938	0.1591	1007.8	1475.0	-0.659	-0.677	-16.7	-16.8	456.1
0.5266	0.1490	1008.6	1477.9	-0.624	-0.639	-16.2	-16.2	454.0
0.5497	0.1468	1010.1	1481.2	-0.615	-0.615	-15.9	-15.9	451.3
0.5801	0.1367	1010.6	1483.5	-0.575	-0.574	-15.2	-15.2	449.6
0.6129	0.1220	1010.5	1484.9	-0.516	-0.522	-14.4	-14.4	448.8
0.6341	0.1200	1011.8	1487.8	-0.501	-0.499	-13.9	-13.9	446.5
0.6531	0.1122	1011.8	1488.7	-0.468	-0.468	-13.4	-13.4	446.0
0.6734	0.1062	1012.2	1490.3	-0.439	-0.439	-12.8	-12.8	444.8
0.6934	0.0993	1012.5	1491.5	-0.407	-0.408	-12.2	-12.2	444.0
0.7124	0.0937	1012.9	1492.9	-0.378	-0.380	-11.6	-11.6	442.9
0.1133	0.2200	986.3	1500.9	-0.076	-0.083	-10.5	-10.0	450.1
0.1460	0.2564	994.7	1513.3	-0.105	-0.104	-11.0	-11.1	439.0
0.1697	0.2434	994.9	1514.5	-0.102	-0.102	-11.3	-11.3	438.2
0.1808	0.2557	997.8	1518.8	-0.114	-0.111	-11.4	-11.7	434.5
0.2004	0.2429	997.7	1519.4	-0.108	-0.106	-11.7	-11.9	434.2
0.2329	0.2361	999.6	1523.3	-0.107	-0.106	-12.2	-12.4	431.1
0.2654	0.5434	1054.6	1593.4	-0.297	-0.323	-9.1	-11.4	373.5
0.2765	0.5365	1054.6	1594.1	-0.301	-0.329	-9.4	-11.4	373.1
0.2891	0.5200	1053.1	1592.9	-0.308	-0.328	-9.8	-11.6	374.2
0.3072	0.5013	1051.7	1592.3	-0.314	-0.329	-10.3	-11.7	375.0
0.3327	0.4823	1051.1	1593.0	-0.320	-0.333	-10.9	-11.6	374.9
0.3501	0.2231	1008.5	1539.9	-0.119	-0.114	-13.5	-13.9	418.2
0.3664	0.4467	1048.4	1591.3	-0.325	-0.325	-11.6	-11.6	376.7
0.3933	0.4187	1046.3	1589.9	-0.324	-0.314	-12.1	-11.6	378.1
0.4018	0.2032	1010.1	1544.0	-0.105	-0.102	-13.8	-14.1	415.3
0.4142	0.4083	1046.6	1591.2	-0.321	-0.315	-12.3	-11.2	377.4
0.4261	0.1838	1009.2	1543.6	-0.080	-0.085	-13.9	-14.1	415.9
0.4299	0.3700	1041.6	1585.2	-0.314	-0.284	-12.8	-11.7	382.0
0.4447	0.1876	1011.6	1547.4	-0.094	-0.093	-14.0	-14.2	412.9
0.4615	0.1765	1011.4	1547.5	-0.081	-0.083	-14.0	-14.2	412.9
0.5003	0.1678	1013.6	1551.5	-0.081	-0.080	-14.0	-14.1	409.8
0.5301	0.1589	1015.0	1554.0	-0.078	-0.075	-13.9	-13.9	408.0
0.5469	0.1487	1014.9	1554.2	-0.066	-0.066	-13.8	-13.8	407.9
0.5763	0.1412	1016.4	1556.6	-0.065	-0.063	-13.6	-13.5	406.0
0.6062	0.1246	1016.5	1557.1	-0.047	-0.048	-13.3	-13.3	405.8
0.6254	0.1227	1018.0	1559.1	-0.053	-0.050	-13.0	-12.9	404.1
0.6550	0.1066	1018.1	1559.4	-0.036	-0.036	-12.6	-12.6	403.9
0.6779	0.1088	1020.7	1562.6	-0.050	-0.045	-12.1	-11.9	401.2
0.6960	0.1020	1021.3	1563.2	-0.045	-0.041	-11.8	-11.5	400.7
0.7151	0.0956	1022.1	1563.9	-0.042	-0.038	-11.3	-11.1	400.0
0.1133	0.2200	982.5	1484.7	-0.143	-0.142	-11.9	-11.4	461.8
0.1460	0.2564	991.1	1496.8	-0.192	-0.182	-12.3	-12.4	450.4
0.1697	0.2434	991.4	1497.7	-0.195	-0.195	-12.6	-12.6	449.7
0.1808	0.2557	994.4	1501.8	-0.213	-0.207	-12.7	-12.9	445.9
0.2004	0.2429	994.2	1502.2	-0.211	-0.213	-12.9	-13.0	445.7
0.2329	0.2361	996.2	1505.7	-0.218	-0.224	-13.1	-13.3	442.8

0.2654	0.5434	1051.1	1575.5	-0.382	-0.401	-9.6	-11.9	383.3
0.2765	0.5365	1051.1	1576.2	-0.387	-0.408	-9.9	-11.9	383.0
0.2891	0.5200	1049.6	1574.9	-0.397	-0.410	-10.3	-12.1	384.2
0.3072	0.5013	1048.2	1574.1	-0.406	-0.414	-10.8	-12.2	385.0
0.3327	0.4823	1047.6	1574.6	-0.412	-0.422	-11.3	-12.1	385.0
0.3501	0.2231	1005.2	1521.0	-0.245	-0.238	-14.0	-14.4	430.0
0.3664	0.4467	1044.9	1572.6	-0.420	-0.420	-12.1	-12.1	387.0
0.3933	0.4187	1042.8	1571.0	-0.422	-0.415	-12.6	-12.0	388.6
0.4018	0.2032	1006.8	1524.6	-0.228	-0.224	-14.1	-14.4	427.3
0.4142	0.4083	1043.1	1572.2	-0.416	-0.419	-12.7	-11.6	387.9
0.4261	0.1838	1005.8	1523.9	-0.198	-0.206	-14.0	-14.2	428.1
0.4299	0.3700	1038.1	1566.1	-0.418	-0.390	-13.2	-12.1	392.7
0.4447	0.1876	1008.2	1527.6	-0.212	-0.209	-14.1	-14.3	425.1
0.4615	0.1765	1007.9	1527.6	-0.194	-0.198	-14.0	-14.2	425.2
0.5003	0.1678	1010.0	1531.3	-0.189	-0.187	-13.9	-14.0	422.2
0.5301	0.1589	1011.3	1533.6	-0.180	-0.176	-13.7	-13.7	420.4
0.5469	0.1487	1011.1	1533.6	-0.163	-0.163	-13.6	-13.6	420.5
0.5763	0.1412	1012.6	1536.0	-0.156	-0.153	-13.3	-13.2	418.6
0.6062	0.1246	1012.5	1536.3	-0.128	-0.130	-12.9	-12.9	418.5
0.6254	0.1227	1014.0	1538.3	-0.130	-0.127	-12.7	-12.5	416.7
0.6550	0.1066	1014.0	1538.4	-0.104	-0.104	-12.2	-12.2	416.7
0.6779	0.1088	1016.5	1541.7	-0.114	-0.109	-11.7	-11.5	413.9
0.6960	0.1020	1017.1	1542.3	-0.104	-0.100	-11.3	-11.1	413.3
0.7151	0.0956	1017.7	1543.1	-0.095	-0.092	-10.9	-10.6	412.7
0.1133	0.2200	978.3	1465.8	-0.206	-0.197	-12.9	-12.4	475.7
0.1460	0.2564	987.2	1477.9	-0.275	-0.256	-13.3	-13.5	463.8
0.1697	0.2434	987.5	1478.6	-0.286	-0.286	-13.5	-13.5	463.2
0.1808	0.2557	990.6	1482.7	-0.310	-0.300	-13.6	-13.8	459.2
0.2004	0.2429	990.5	1482.9	-0.313	-0.318	-13.7	-13.8	459.1
0.2329	0.2361	992.6	1486.1	-0.328	-0.340	-13.9	-14.0	456.2
0.2654	0.5434	1047.5	1557.2	-0.462	-0.470	-10.4	-12.5	393.7
0.2765	0.5365	1047.5	1557.7	-0.466	-0.478	-10.7	-12.5	393.4
0.2891	0.5200	1046.0	1556.3	-0.479	-0.483	-11.1	-12.7	394.7
0.3072	0.5013	1044.6	1555.4	-0.490	-0.491	-11.5	-12.8	395.7
0.3327	0.4823	1044.0	1555.7	-0.496	-0.503	-12.0	-12.7	395.8
0.3501	0.2231	1001.8	1500.8	-0.372	-0.363	-14.4	-14.7	443.2
0.3664	0.4467	1041.3	1553.5	-0.508	-0.508	-12.7	-12.7	397.9
0.3933	0.4187	1039.2	1551.7	-0.513	-0.508	-13.1	-12.6	399.6
0.4018	0.2032	1003.3	1504.0	-0.353	-0.349	-14.3	-14.6	440.6
0.4142	0.4083	1039.4	1552.8	-0.504	-0.515	-13.1	-12.1	399.0
0.4261	0.1838	1002.2	1503.1	-0.319	-0.332	-14.1	-14.3	441.6
0.4299	0.3700	1034.6	1546.7	-0.517	-0.490	-13.8	-12.6	404.1
0.4447	0.1876	1004.7	1506.8	-0.333	-0.330	-14.2	-14.3	438.4
0.4615	0.1765	1004.3	1506.7	-0.312	-0.317	-14.0	-14.2	438.6
0.5003	0.1678	1006.4	1510.4	-0.301	-0.298	-13.8	-13.9	435.6
0.5301	0.1589	1007.6	1512.6	-0.286	-0.281	-13.6	-13.6	433.8
0.5469	0.1487	1007.4	1512.5	-0.265	-0.265	-13.4	-13.4	433.9
0.5763	0.1412	1008.8	1514.9	-0.252	-0.248	-13.1	-13.0	431.9
0.6062	0.1246	1008.7	1515.1	-0.216	-0.217	-12.6	-12.6	431.9
0.6254	0.1227	1010.1	1517.2	-0.213	-0.210	-12.3	-12.2	430.1
0.6550	0.1066	1010.0	1517.3	-0.178	-0.178	-11.8	-11.8	430.1
0.6779	0.1088	1012.5	1520.7	-0.184	-0.179	-11.4	-11.1	427.1
0.6960	0.1020	1013.0	1521.4	-0.169	-0.165	-11.0	-10.7	426.5
0.7151	0.0956	1013.6	1522.2	-0.155	-0.151	-10.5	-10.3	425.8
0.1133	0.2200	974.0	1446.6	-0.2656	-0.2483	-13.8	-13.5	490.6
0.1460	0.2564	983.1	1458.9	-0.3535	-0.3259	-14.4	-14.5	477.9
0.1697	0.2434	983.5	1459.3	-0.3720	-0.3720	-14.4	-14.4	477.5
0.1808	0.2557	986.6	1463.5	-0.4019	-0.3885	-14.6	-14.8	473.2
0.2004	0.2429	986.6	1463.4	-0.4089	-0.4167	-14.6	-14.7	473.3
0.2329	0.2361	988.7	1466.4	-0.4327	-0.4504	-14.7	-14.8	470.3
0.2654	0.5434	1043.6	1539.8	-0.5311	-0.5285	-11.4	-13.4	404.1
0.2765	0.5365	1043.5	1540.3	-0.5349	-0.5370	-11.6	-13.4	403.9
0.2891	0.5200	1042.1	1538.7	-0.5502	-0.5454	-12.0	-13.6	405.3
0.3072	0.5013	1040.7	1537.7	-0.5636	-0.5566	-12.5	-13.7	406.4

0.3327	0.4823	1040.0	1537.7	-0.5692	-0.5724	-12.8	-13.6	406.6
0.3501	0.2231	998.1	1480.5	-0.4932	-0.4824	-14.9	-15.2	457.1
0.3664	0.4467	1037.3	1535.3	-0.5851	-0.5851	-13.5	-13.5	409.0
0.3933	0.4187	1035.2	1533.3	-0.5920	-0.5902	-13.9	-13.4	410.9
0.4018	0.2032	999.5	1483.4	-0.4725	-0.4673	-14.7	-14.9	454.6
0.4142	0.4083	1035.4	1534.2	-0.5804	-0.6001	-13.9	-13.0	410.3
0.4261	0.1838	998.4	1482.2	-0.4345	-0.4529	-14.3	-14.5	455.9
0.4299	0.3700	1030.6	1527.9	-0.6034	-0.5794	-14.6	-13.4	415.6
0.4447	0.1876	1000.8	1486.0	-0.4485	-0.4448	-14.4	-14.5	452.5
0.4615	0.1765	1000.4	1485.7	-0.4250	-0.4318	-14.1	-14.3	452.9
0.5003	0.1678	1002.5	1489.3	-0.4092	-0.4056	-13.9	-13.9	449.7
0.5301	0.1589	1003.6	1491.5	-0.3891	-0.3824	-13.6	-13.6	447.9
0.5469	0.1487	1003.3	1491.3	-0.3637	-0.3637	-13.3	-13.3	448.1
0.5763	0.1412	1004.7	1493.7	-0.3445	-0.3395	-13.0	-12.9	446.1
0.6062	0.1246	1004.4	1493.7	-0.3004	-0.3025	-12.4	-12.4	446.2
0.6254	0.1227	1005.8	1496.0	-0.2943	-0.2901	-12.2	-12.0	444.3
0.6550	0.1066	1005.5	1495.9	-0.2502	-0.2502	-11.5	-11.5	444.4
0.6779	0.1088	1008.0	1499.6	-0.2527	-0.2462	-11.2	-10.9	441.1
0.6960	0.1020	1008.4	1500.3	-0.2330	-0.2275	-10.8	-10.5	440.6
0.7151	0.0956	1009.0	1501.1	-0.2141	-0.2095	-10.3	-10.0	439.8

Table 3 Ternary adjustable parameters, $Y_{123}^{(n)}$ (Y= V or κ_S; n = 0-2) of Eq. (5) along with their standard deviations, $\sigma(Y^E)(Y = V or\ \kappa_S)$ of V_{123}^E and $\left(\kappa_S^E\right)_{123}$ at T = (293.15, 298.15, 303.15, 308.15) K

Parameters	T/K			
	293.15	298.15	303.15	308.15
N-Methylpyrrolidin-2-one (1) + Pyrrolidin-2-one (2) + Cyclopentanone (3)				
$V^{(0)}$	-12.613	-15.723	-19.312	-21.513
$V^{(1)}$	-38.921	-34.501	-27.543	-19.827
$V^{(2)}$	98.416	125.496	187.322	217.232
$\sigma(V_{123}^E)$ /cm^{-3}·mol^{-1}	0.001	0.001	0.001	0.001
$\kappa_S^{(0)}$	-25.8	-36.4	-46.2	-63.7
$\kappa_S^{(1)}$	-312.8	-292.8	-271.3	-254.5
$\kappa_S^{(2)}$	657.3	1214.5	2372.3	3466.6
$\sigma\left(\kappa_S^E\right)_{123}$ /TPa^{-1}	0.4	0.4	0.5	0.5
N-Methylpyrrolidin-2-one (1) + Pyrrolidin-2-one (2) + Cyclohexanone (3)				
$V^{(0)}$	-9.5	-20.2	-29.9	-47.7
$V^{(1)}$	-274.2	-254.3	-232.3	-215.3
$V^{(2)}$	767.4	1325.0	2427.7	3611.4
$\sigma(V_{123}^E)$ /cm^{-3}·mol^{-1}	0.001	0.001	0.001	0.001
$\kappa_S^{(0)}$	537.83	502.49	443.04	292.05
$\kappa_S^{(1)}$	8009.35	7694.89	9533.36	9929.07
$\kappa_S^{(2)}$	30005.88	29904.62	46528.48	56825.22
$\sigma\left(\kappa_S^E\right)_{123}$ /TPa^{-1}	0.3	0.3	0.4	0.4

Table 4

Interaction energies χ^*, $\chi_{12}^{/}$; $\chi_{12}^{//}$; $\chi_{12}^{///}$ etc. parameters along with connectivity parameters of third degree of a molecule, $(^3\xi_1)$ or $(^3\xi_2)_m$ (1 = 1 or 2 or 3) utilized for the determination of V_{123}^E and $(\kappa_S^E)_{123}$ at T = (293.15, 298.15, 303.15, 308.15) K. Also included are the standard deviations between the experimental data and the values calculated by various theories.

Parameters	T/K

	293.15	298.15	303.15	308.15
N-Methyl-2-pyrrolidone (1) + Pyrrolidin-2-one (2) + Cyclopentanone (3)				
$({}^3\xi_1) = ({}^3\xi_1)_m$	1.016	1.016	1.016	1.016
$({}^3\xi_2) = ({}^3\xi_2)_m$	1.203	1.203	1.203	1.203
$({}^3\xi_3) = ({}^3\xi_3)_m$	1.270	1.270	1.270	1.270
χ'_{12} /cm^3·mol^{-1}	-1.702	-1.438	-1.041	-0.617
χ'_{23} /cm^3· mol^{-1}	0.187	0.504	0.834	1.156
χ'_{13} /cm^3 ·mol^{-1}	0.123	0.272	0.422	0.554
χ^* /cm^3 ·mol^{-1}	-1.461	-3.056	-4.861	-6.510
σ ($V^E_{123\ Graph}$)	0.009	0.009	0.010	0.012
χ'_{12} /TPa^{-1}	-25.6	-25.1	-26.0	-30.1
χ'_{23} /TPa^{-1}	-16.5	-21.1	-27.9	-36.0
χ'_{13} /TPa^{-1}	-13.2	-15.5	-18.8	-24.3
χ^* /TPa^{-1}	-14.1	-16.7	-11.1	2.3
σ ((κ^E_S)$_{123\ Graph}$)	0.1	0.2	0.2	0.3
N-Methyl-2-pydrrolidone (1) + Pyrrolidin-2-one (2) + Cyclohexanone (3)				
$({}^3\xi_1) = ({}^3\xi_1)_m$	1.012	1.012	1.012	1.012
$({}^3\xi_2) = ({}^3\xi_2)_m$	0.666	0.666	0.666	0.666
$({}^3\xi_3) = ({}^3\xi_3)_m$	1.182	1.182	1.182	1.182
χ'_{12} /cm^3·mol^{-1}	5.407	7.891	10.091	12.610
χ'_{23} /cm^3· mol^{-1}	3.567	4.819	5.938	7.215
χ'_{13} /cm^3 ·mol^{-1}	1.387	2.460	3.421	4.518
χ^* /cm^3 ·mol^{-1}	-13.351	-18.815	-23.694	-29.261
σ ($V^E_{123\ Graph}$)	0.010	0.007	0.010	0.017
χ'_{12} /TPa^{-1}	31.66	111.16	110.73	181.67
χ'_{23} /TPa^{-1}	73.27	111.06	106.73	137.66
χ'_{13} /TPa^{-1}	10.70	45.74	59.05	103.91
χ^* /TPa^{-1}	-203.27	-380.20	-409.67	-595.82
σ ((κ^E_S)$_{123\ Graph}$)	0.28	0.16	0.15	0.51