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Study on Interaction Capabilities of Ternary Liquid Mixtures by Thermodynamic Parameters at 308.15 K

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Abstract

Thermodynamic properties provide a deep and significant insight of the various interactions taking place multi component liquid mixtures especially in the field of petrochemical and reservoir engineering. The density, viscosity and ultrasonic velocity were measured experimentally for diethylmalonate (DEM) +1,4-dioxane with nitrobenzene (TM-1) and diethylmalonate (DEM) +1,4-dioxane + toluene (TM-2) at the temperature of 308.15K and atmospheric pressure over the entire range of mole fraction. The excess thermodynamic properties such as excess volume (V^E), excess adiabatic compressibility (ΔK_s), excess viscosity ($\Delta\eta$), excess free volume (ΔV_F), excess free length (ΔL_F), excess isothermal compressibility ($\Delta\beta_T$), were calculated from measured values and applied to Redlich - Kister polynomial equation to determine the appropriate coefficients. The excess or deviation properties were found to be either negative or positive depending on the molecular interactions and the nature of liquid mixtures. The deviations of the ternary mixtures from its ideal behaviour were determined in order to investigate the molecular interaction between the components of ternary liquid mixtures.

Keywords: *Mole fractions; ternary liquid mixtures; structural activities; Redlich - Kister polynomial equation; molecular interactions.*

1. Introduction

Many fields such as pharmaceuticals, petroleum and chemical engineering require information regarding thermodynamic properties of the liquid mixtures. The study of transport fluid phenomena entails the data regarding density and viscosity of the system [1] Other than density and viscosity the ultrasonic study provides huge data about the molecular interactions [2] and the structural activities of the molecules in the mixture. The variation in thermodynamic and transport properties of liquid mixtures from its pure constituents is a energetic tool to study the nature of molecular interactions (either intermolecular or intramolecular) between mixing liquids. The study of physical properties like density, viscosity, excess molar volume, volume fraction and adiabatic compressibility aid in understanding the nature and strength of intra and intermolecular interactions occurring in multi component liquid systems[3]. Also the thermodynamic and transport properties of liquid systems are vital for engineering process design and operation. There are several predictive equations for estimating thermodynamic properties. The thermodynamic properties of organic liquids help in separation of organic liquid mixtures through fractional distillation which can be helpful to reduce pollution of environment. In the present work, a binary mixture of diethylmalonate (DEM) + 1,4- dioxane or p-dioxane has been used to prepare ternary solutions by adding nitrobenzene and toluene separately [4-8]. The thermodynamic and transport properties of prepared ternary solutions have been studied at 308.15 K and 318.15K over a wide range of compositions. The investigated properties such as excess volume, viscosity, adiabatic compressibility, free length, free volume and isentropic compressibility can be used to parameterize the energy transfer process and interactions between the ternary mixtures. Therefore the detailed study of the thermodynamic and transport properties of the ternary mixtures of diethylmalonate (1) + 1,4-dioxane (2) with nitrobenzene (3) and toluene (3) at 308.15 hence form the main scope of the present work.

2. Materials and Methods

Diethylmalonate and 1,4 dioxane (Merck, Mumbai, India), nitrobenzene and toluene (Loba, Mumbai, India), all Analar grades with 99% pure. All the chemicals used were directly purchased from the producers and purified by double distillation method. Hence the techniques to ascertain purity are not attempted but the measured densities, viscosities, and ultrasonic velocities were confirmed by comparing with earlier literature reports in Table1. Ternary liquid mixtures were prepared by weight by volume in airtight stoppered bottles using an analytical balance with an accuracy of ±±0.1 mg. Densities of pure liquids and their mixtures were measured using relative density method. Relative density bottle of 10ml capacity

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was cleaned successively with chromic acid, distilled water and acetone and then dried and used for density measurements [10]. An electronic balance was used to measure the density [11]. The accuracy of the measurement of density in relative density method depends on the accuracy of mass. Density values are accurate to ±0.0002 gcm^{-3}. Viscosities were measured using an Ostwald. viscometer. Viscometer was thoroughly cleaned with chromic acid. An electronic digital stopwatch with readability of ±0.01 s was used to measure the flow time of liquid between the marks. The ultrasonic velocity values were measured using an ultrasonic interferometer (Pico, Chennai, India) with a frequency of 2MHz was calibrated using water and nitrobenzene. The overall accuracy in the measurement is ±0.2%. All the measurements were made using a digital thermostat which displays accuracy ±0.01 K. The details of the methods and techniques of the measurements have been described earlier [12, 13]. The following are the equations used in calculating thermodynamic parameters nitrobenzene (3) and toluene (3) at 308.15 hence form the main scope of the present work.
The excess volume values for the ternary mixtures were calculated using the relation.

$$V^E=\left(\frac{X_1M_1+X_2M_2+X_3M_3}{\rho_{mix}}\right)-\left(\frac{X_1M_1}{\rho_1}\right)-\left(\frac{X_2M_2}{\rho_2}\right)-\left(\frac{X_3M_3}{\rho_3}\right) \qquad (1)$$

where X_1, X_2 & X_3, M_1, M_2 & M_3 and ρ_1, ρ_2 & ρ_3 are the mole fractions, molar mass, densities of pure components 1, 2, 3 respectively.
Adiabatic compressibility (K_s) has been calculated from Laplace's equation [14]

$$K_s=\frac{1}{\rho U^2} \qquad (2)$$

Where ρ and U are the density and ultrasonic velocity of liquid mixtures. From the above equation excess adiabatic compressibility (ΔK_S) has been calculated by

$$K_S=K_S-\phi_1K_{S1}-\phi_2K_{S2}-\phi_3K_{S3} \qquad (3)$$

K_{S1}, K_{S2}, K_{S3} are adiabatic compressibility of pure liquids and ϕ_1, ϕ_2, ϕ_3 are the volume fractions of pure liquids calculated by the relation

$$\phi_1=\frac{\left(\frac{X_1M_1}{\rho_1}\right)}{\left(\frac{X_1M_1}{\rho_1}+\frac{X_2M_2}{\rho_2}+\frac{X_3M_3}{\rho_3}\right)} \qquad (4)$$

Viscosity has been calculated using the relation

$$\eta=\left(At-\frac{B}{t}\right)\rho \qquad (5)$$

A and B are the constant characteristics of viscometer calculated using the standard liquids water and nitrobenzene, t is the flow time, ρ is the density.
Excess viscosity values are calculated using the following relation

$$\Delta\eta=\eta-(X_1\eta_1+X_2\eta_2+X_3\eta_3) \qquad (6)$$

Where η_1 and η_2 are the viscosity values of pure components 1 and 2 respectively.
Free length is calculated using the relation,

$$L_f=\frac{K}{up^{1/2}} \qquad (7)$$

K is Jacobson's [15] constant, which is temperature dependent constant but independent of the nature of the liquid.
Isothermal compressibility is calculated using the relation.

$$\beta_T=\frac{1.71\times10^{-3}}{\left(\frac{T^4}{9u^2\rho^{\frac{4}{3}}}\right)} \qquad (8)$$

A relation to calculate free volume is [16]

$$V_f=\left(\frac{M_{eff}u}{K\eta}\right)^{\frac{3}{2}} \qquad (9)$$

K is a temperature independent constant which is equal to 4.28x10^9 for all the liquids; M_{eff} is effective molecular weight of the mixture calculated using the relation.

$$M_{eff}=X_1M_1+X_2M_2+X_3M_3 \qquad (10)$$

Where X_1, X_2, X_3 and M_1, M_2, M_3 are the mole fractions and molar mass of pure components 1, 2, 3 respectively.
Excess values of other parameters are calculated using the relation

$$A^E=A_{exp}-A_{id}$$
$$A_{id}=\Sigma X_iA_i \qquad (11)$$

Where X_i and A_i are mole fraction and parameters of the ith component.
All the calculated excess parameters are fitted to Redlich–Kister [17] type polynomial equation by the method of least squares to derive the adjustable parameters a, b, c.
For binary

$$A^E=\left[X_1X_2\left(a+b(X_1-X_2)+c(X_1-X_2)\right)\right] \qquad (12)$$

For ternary

$$A^E=[X_1X_2X_3(a+bX_1(X_2-X_3)+cX_1^2(X_2-X_3)^2)] \qquad (13)$$

Using the theoretical values for all excess parameters were calculated and the standard deviation values were calculated using the relation

$$\sigma=\left[\frac{\left(A_{exp}-A_{cal}\right)^2}{(n-m)}\right]^{\frac{1}{2}} \qquad (14)$$

n is the number of measurements and m is the number of adjustable parameters.1,4-dioxane could be classified as a non- polar solvent, but the distribution of electric charge gives a large quadruple moment to 1,4-dioxane[18]. The presence of substituent in the aromatic hydrocarbon should modulate its electron-acceptor ability [19]. In diethylmalonate there are two types of molecular surface, the non- polar ethyl group and the polar carboxyl residues –COO-[20]. Nitrobenzene is an aromatic hydrocarbon containing NO2 as a functional group. The electron withdrawing -NO2 group draws π- electrons from the aromatic electron cloud of benzene generating a $\delta+$ charge in it. Hence the mode of self-interaction in nitrobenzene is the potential anionic - π stacking interaction possible through the nucleophilic oxygen atom of the –NO2 group with the generated $\delta+$ charge of the aromatic π electron cloud of benzene moiety [21]. Toluene, a methyl carrying benzene ring in which the methyl releases electron to the benzene moiety.

3. Results and Discussion

The ternary liquid solutions have been prepared by mixing diethylmalonate (1) +1,4-dioxane (2) with nitrobenzene (3) and toluene (3) varying their mole fractions. Experimental densities, viscosity, ultrasonic velocities of pure components of the liquid mixture were compared with literature values and are reported in Table 1. Also their excess thermodynamic parameters have been calculated and tabulated at a temperature of 308.15K to understand the interactions possible between them.

Calculated thermodynamic parameters and excess acoustical parameters for the ternary liquid mixtures of diethylmalonate(1) + 1, 4-dioxane(2) with nitrobenzene(3) and toluene(3) are represented in table 2 and table 3 respectively.

The greater interaction in the ternary system results in volume contraction in the system containing nitrobenzene as one of the component are indicated by the negative V^E values for the entire mole fractions at 308.15K. When comparing the corresponding binaries the V^E the interaction between the p-dioxane and nitrobenzene is lower than DEM and nitrobenzene. The values of ΔKs are directly proportional to different size and shape of the components and inversely proportional to velocity. Also ΔKs vary due to change in free volume. The ΔK_s values are negative for the considered mole fractions at 308.15. The negative values of ΔK_s clearly indicate the presence of molecular interactions and which make the flexible and more compressible. The deviation in viscosity values are low positive for maximum mole fractions at 308.15K may designate that the interaction between the component molecules are higher. The ΔL_F values are also negative may indicate the existence of interactions between the component molecules. The viscosity of a mixture depends on the molecular interaction between the components of the liquid mixtures. Components showing strong interactions are indicated by the positive deviations of viscosity. The viscosity deviation values indicate the existence of interaction between the component molecules values of the considered ternary mixture is greater and the prediction is supported by V^E and ΔKs values. The deviation in isothermal compressibility and thermal expansion coefficient are negative. The negative values may clearly indicate the greater interstitial accommodation of the molecules to each other. The deviation of the free volume for the considered ternary mixture shows negative deviations for the entire mole fractions also supports the above predictions. The greater interactions between the mixing components in the ternary systems results in negative deviation values and the positive values may indicate the existence of weak interactions.

The calculated thermodynamic properties for the considered binary liquid mixtures of diethylmalonate + p-dioxane + toluene are tabulated in Table 3 for 308.15K. The V^E values for the ternary mixtures of diethylmalonate + p-dioxane + toluene shows positive values at 308.15K. The positive values are due to the presence of weak Vander Waals force existing between the molecules of ternary system. The weak Vander Waals force between the molecules of ternary system may make the system very slightly compressible and somewhat flexible which is indicated by low positive and low negative values of ΔKs. The compactness of the system is clearly designated by free length, ΔL_F values are positive. The viscosity deviations values shown by maximum number of mole fractions are negative at 308.15 K, due to the presence of weak forces existing between the component molecules. The deviation in isothermal compressibility $\Delta \beta_T$ is low negative values may be due to the better interstitial accommodation of the molecules where the prediction supports the viscosity deviation values.

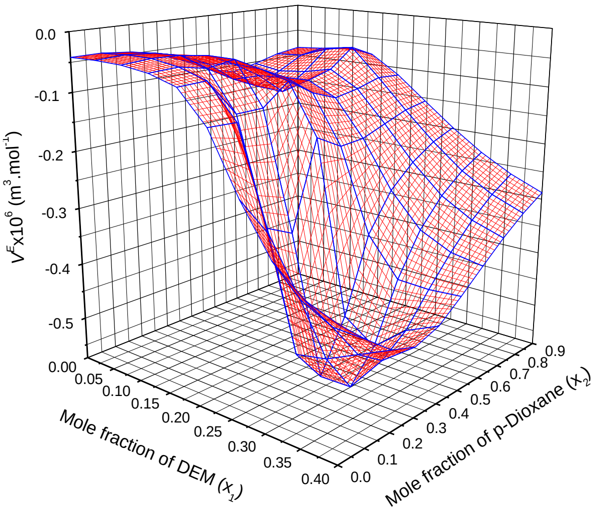

Figure 1. V^E versus mole fractions plots for TM1.

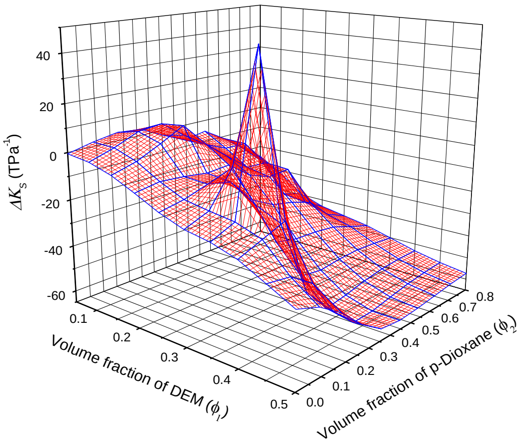

Figure 2. ΔK_s versus volume fraction plots for TM 1.

The ΔV_F value is negative is due to the presence of weak force of attraction between the molecules of the system. The calculated excess thermodynamic parameters were fitted to Redlich – Kister polynomial equation to determine the adjustable coefficients and tabulated in Table 4 and Table 5 for DEM (1) + p-dioxane (2) and nitrobenzene(3) and toluene(3) respectively.

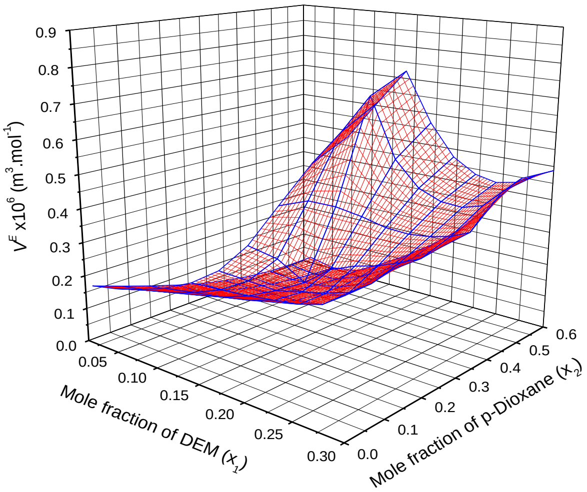

Figure 3. V^E versus mole fractions plots for TM 2.

Figure 1 and 3 represents 3D schematic diagrams of excess volume (V^E) of nitrobenzene and toluene versus mole fractions plots for DEM (X_1).

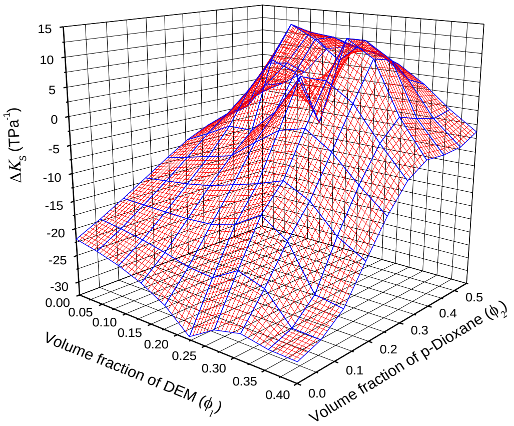

Figure 4. ΔK_s versus volume fraction plots for TM 2.

p-dioxane (X_2) respectively. Figure 2 and 4 represents 3D schematic diagrams of adiabatic compressibility (ΔK_s) of nitrobenzene and toluene versus volume fractions plots for DEM (φ_1) + p-dioxane (φ_2) at 308.15K and 318.15K respectively.

4. Conclusion

The densities, ultrasonic velocities, viscosities have been measured for the two ternary mixtures of diethylmalonate +1,4-dioxane + nitrobenzene and morpholine+1,4-dioxane + toluene and other excess thermodynamic properties such as excess volume, adiabatic compressibility, deviation in viscosity, free length, isothermal compressibility, free volume for have been calculated at atmospheric pressures and at the temperature of 308.15 K. The relevant values for pure components of the mixtures are also provided for reference. The corresponding thermodynamic excess parameters were calculated with the formulas reported earlier and fitted to a Redlich – Kister type polynomial equation to determine the adjustable coefficients. The behaviour of the liquid mixtures and the deviation from the ideal behaviour has been discussed based on experimental and calculated values. The V^E values suggest that existence of inter-molecular interactions between the component molecules in the liquid mixtures of diethylmalonate + p-dioxane wit nitrobenzene is higher than with toluene. The intermolecular interactions may make diethylmalonate + 1,4-dioxane + nitrobenzene mixture slightly flexible and little compressible indicated by its ΔKs values. On contrast the ΔKs values of diethylmalonate +1,4-dioxane + toluene mixture suggests the possibility for the occurrence of stiffness and less compressible nature. Both the ternary mixtures exhibit intermolecular interactions between like molecules. All the other calculated thermodynamic parameters supports the above predictions. The self-interaction may prevalent in ternary mixture containing nitrobenzene, and it may become less significant for the ternary mixture associated with toluene. According to the measured and calculated properties it can be assumed that strong molecular interactions is possible in diethylmalonate + 1,4-dioxane + nitrobenzene than diethylmalonate + 1,4-dioxane + toluene.

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Nomenclature:

V^E	Excess volume
K_s	Adiabatic compressibility
K	Jacobson's constant
X_i	Mole fraction of the ith component.
A_i	Parameters of the ith component. (Redlich–Kister equation Coefficients)
ρ_{mix}	Density of liquid mixture
n	Number of measurements
m	Number of adjustable parameters
t	Flow time

Appendix

Table 1. Densities (ρ), viscosities (η) and ultrasonic velocities (U) of pure diethylmalonate, 1,4- dioxane nitrobenzene and toluene at 308.15K.

Compounds	T/K	ρ x 10^{-3} / kgm^{-3}		η / cP		U / ms^{-1}	
		Exp	Lit	Exp	Lit	Exp	Lit
Diethylmalonate[4]	308.15	1.032	1.0387	1.2754	1.2672	1258	-
Nitrobenzene[22]	308.15	1.1877	1.1911	1.5678	1.5543	1375	1379
1,4-dioxane[23,24]	308.15	1.0167	1.0166	1.025	1.0280	1300	1300.3
Toluene[25,26]	308.15	0.8378	0.8566*	0.5099	0.5270*	1250	-

* refers to values at 303.15 K

Table 2. Values of thermodynamic properties of TM 1 ternary liquid mixture at 308.15K.

X_1	X_2	$\rho x10^{-3}$/ kgm^{-3}	V^E x 10^6/ m^3mol^{-1}	U/ ms^{-1}	ϕ_1	ϕ_2	ΔK_s / TPa^{-1}
0.0315	0.4800	1.1081	-0.0992	1340	0.0500	0.4285	-8.9827
0.0445	0.5263	1.0981	-0.1252	1330	0.0709	0.4704	-5.8929
0.0363	0.5451	1.0966	-0.1358	1324	0.0582	0.4911	-0.7401
0.1030	0.5693	1.0798	-0.0977	1330	0.1602	0.4975	-14.3211
0.0752	0.6958	1.0630	-0.1097	1318	0.1213	0.6306	-8.4314
0.0840	0.6218	1.0749	-0.1582	1338	0.1332	0.5537	-21.8074
0.1522	0.3626	1.1039	-0.0570	1318	0.2232	0.2988	0.9901
0.0953	0.2946	1.1248	-0.0456	1312	0.1421	0.2468	15.5596
0.0961	0.7914	1.0418	-0.0679	1352	0.1560	0.7215	-42.1416
0.1106	0.8013	1.0374	-0.0441	1346	0.1784	0.7261	-39.2197
0.1319	0.7323	1.0467	-0.0841	1318	0.2079	0.6484	-16.2031
0.1357	0.2957	1.1171	-0.0474	1350	0.1984	0.2430	-17.5995
0.1406	0.7591	1.0403	-0.0579	1350	0.2216	0.6723	-43.5497
0.1569	0.4111	1.0960	-0.0979	1335	0.2314	0.3406	-15.9636
0.1636	0.7655	1.0360	-0.0976	1336	0.2551	0.6707	-35.4932
0.1858	0.4119	1.0907	-0.0862	1346	0.2703	0.3366	-26.4027
0.2103	0.0964	1.1325	-0.0446	1354	0.2880	0.0742	-18.4343
0.2107	0.3960	1.0884	-0.0336	1356	0.3022	0.3191	-35.9233
0.2587	0.1774	1.1157	-0.3547	1336	0.3509	0.1352	-15.4330
0.2424	0.3816	1.0891	-0.4081	1358	0.3417	0.3022	-41.7232
0.2564	0.2254	1.1123	-0.6643	1370	0.3507	0.1732	56.4284
0.2930	0.3729	1.0842	-0.6119	1380	0.4030	0.2883	-62.2624
0.3083	0.3930	1.0779	-0.5193	1372	0.4224	0.3026	-59.2086
0.3520	0.4392	1.0636	-0.4382	1367	0.4763	0.3339	-60.7545

Table 2. Continued…………..

X_1	X_2	η cP	$\Delta\eta$ cP	ΔL_F x10^{-10}/ M	$\Delta\beta_T$ x10^{-12}/ $kg^{-1}K^{-1}m^2s$	ΔV_F x 10^{-10}/ m^3mol^{-1}
0.0315	0.4800	1.3146	0.0129	-2.0967	-2.2907	-1.3218
0.0445	0.5263	1.2035	-0.0706	-1.8973	-1.7605	-1.3348
0.0363	0.5451	1.2763	0.0109	-1.8137	-1.2117	-1.3298
0.1030	0.5693	1.2323	-0.0071	-1.7379	-2.5441	-1.3819
0.0752	0.6958	1.1891	0.0128	-1.4130	-1.8271	-1.3693
0.0840	0.6218	1.2558	0.0412	-1.7578	-3.6844	-1.3711
0.1522	0.3626	1.1847	-0.1574	-1.8971	7.2852	-1.4055
0.0953	0.2946	1.1814	-0.2085	-2.0194	1.8534	-1.3579
0.0961	0.7914	1.3058	0.1854	-1.5556	-6.2589	-1.3915
0.1106	0.8013	1.3096	0.1973	-1.4520	-5.7575	-1.4031
0.1319	0.7323	1.1233	-0.0222	-1.2637	-2.4619	-1.4147
0.1357	0.2957	1.3852	0.0037	-2.3542	-2.4340	-1.3885
0.1406	0.7591	1.2714	0.1421	-1.5409	-6.2577	-1.4230
0.1569	0.4111	1.3247	0.0099	-1.9926	-2.2572	-1.4123
0.1636	0.7655	1.1823	0.0609	-1.3551	-4.9915	-1.4409
0.1858	0.4119	1.3135	0.0046	-2.0671	-3.6750	-1.4342
0.2103	0.0964	1.4397	-0.0355	-2.5995	-1.3892	-1.4318
0.2107	0.3960	1.3885	0.0758	-2.1596	-4.7531	-1.4521
0.2587	0.1774	1.4753	0.0533	-2.2663	-1.2557	-1.4739
0.2424	0.3816	1.4421	0.1276	-2.1968	-5.4598	-1.4751
0.2564	0.2254	1.5175	0.1211	-2.5612	-5.3632	-1.4754
0.2930	0.3729	1.4552	0.1459	-2.3869	-8.2573	-1.5128
0.3083	0.3930	1.4325	0.1369	-2.2518	-7.7740	-1.5258
0.3520	0.4392	1.4088	0.1467	-2.0731	-8.1429	-1.5620

Table 3. Values of thermodynamic properties of TM 1 ternary liquid mixture at 308.15K.

X_1	X_2	ρx10^{-3}/ kgm^{-3}	V^Ex 10^6/ m^3mol^{-1}	U/ ms^{-1}	ϕ_1	ϕ_2	ΔK_S/ TPa^{-1}
0.0287	0.5220	0.9283	0.0201	1270	0.0447	0.4566	-5.5670
0.0454	0.5708	0.9416	0.0193	1256	0.0710	0.5013	12.8820
0.0470	0.5743	0.9428	-0.0021	1276	0.0734	0.5044	-8.1611
0.0695	0.5936	0.9523	-0.0057	1262	0.1080	0.5186	8.0889
0.0686	0.5487	0.9439	-0.0025	1258	0.1056	0.4745	9.6732
0.0807	0.5283	0.9433	0.0153	1254	0.1230	0.4523	13.4806
0.0994	0.4731	0.9383	0.0278	1250	0.1484	0.3967	15.5374
0.1003	0.4281	0.9308	0.0360	1256	0.1481	0.3552	6.9368
0.1041	0.3855	0.9245	0.0493	1266	0.1521	0.3164	-6.4699
0.1449	0.3621	0.9309	0.0584	1254	0.2070	0.2907	6.8564
0.1377	0.3160	0.9215	0.0687	1260	0.1953	0.2520	-2.1055
0.1591	0.2911	0.9226	0.0985	1264	0.2227	0.2288	-6.8384

0.1578	0.4517	0.9487	0.0899	1270	0.2287	0.3678	-5.5527
0.1638	0.3533	0.9338	0.0898	1252	0.2318	0.2809	9.1343
0.1755	0.0090	0.8827	0.3321	1280	0.2302	0.0066	-33.0351
0.1853	0.4734	0.9582	0.1828	1250	0.2668	0.3829	17.4318
0.2119	0.4914	0.9674	0.1993	1255	0.3029	0.3946	14.4956
0.2188	0.1316	0.9112	0.2800	1264	0.2894	0.0978	11.7303
0.2371	0.5305	0.9793	0.2731	1270	0.3382	0.4253	2.8790
0.2411	0.5656	0.9856	0.3535	1276	0.3460	0.4561	-0.2428
0.2689	0.5736	0.9922	0.4703	1284	0.3823	0.4582	-5.9190
0.2831	0.1938	0.9323	0.6596	1280	0.3700	0.1424	22.4068
0.2931	0.1471	0.9259	0.8883	1284	0.3782	0.1066	26.5679
0.2618	0.1318	0.9173	0.7924	1282	0.3407	0.0964	26.5710

Table 3. Continued……………..

X_1	X_2	η/ cP	$\Delta\eta$/ cP	ΔL_Fx10^{-10}/ M	$\Delta\beta_T$ x10^{-12}/ $kg^{-1}K^{-1}m^2s$	ΔV_F x10^{-10}/ m^3mol^{-1}
0.0287	0.5220	0.7662	-0.1148	-9.7436	-1.2275	-6.2006
0.0454	0.5708	0.7053	-0.1978	-9.4891	-1.2034	-5.0628
0.0470	0.5743	0.8021	-0.1028	-9.4965	-1.2016	-6.1760
0.0695	0.5936	0.8244	-0.0980	-9.3309	-1.1861	-6.2579
0.0686	0.5487	0.8067	-0.1033	-9.4946	-1.2029	-6.3753
0.0807	0.5283	0.7539	-0.1574	-9.5237	-1.2059	-5.8387
0.0994	0.4731	0.6614	-0.2454	-9.6588	-1.2193	-4.6816
0.1003	0.4281	0.6827	-0.2126	-9.8301	-1.2355	-5.294
0.1041	0.3855	0.7085	-0.1776	-9.9871	-1.2498	-5.9004
0.1449	0.3621	0.7318	-0.1705	-9.9198	-1.2433	-6.2602
0.1377	0.3160	0.6993	-0.1868	-10.1231	-1.2629	-6.0419
0.1591	0.2911	0.7138	-0.1774	-10.1473	-1.2641	-6.2959
0.1578	0.4517	0.7236	-0.2095	-9.5640	-1.2056	-5.4184
0.1638	0.3533	0.7313	-0.1790	-9.8853	-1.2395	-6.2243
0.1755	0.0090	1.1564	0.3312	-11.1510	-1.3619	-11.9368
0.1853	0.4734	0.6273	-0.3267	-9.3638	-1.1874	-3.4775
0.2119	0.4914	0.6607	-0.3127	-9.2124	-1.1709	-3.8691
0.2188	0.1316	1.0626	0.1810	-10.5343	-1.3007	-10.5621
0.2371	0.5305	1.0760	0.0782	-8.9989	-1.1472	-8.0226
0.2411	0.5656	1.0751	0.0659	-8.8619	-1.1328	-7.7616
0.2689	0.5736	1.0879	0.0612	-8.7448	-1.1195	-7.6788
0.2831	0.1938	1.1050	0.1715	-10.1013	-1.2540	-10.1811
0.2931	0.1471	1.1508	0.2243	-10.2449	-1.2675	-1.0698
0.2618	0.1318	1.1430	0.2377	-10.4063	-1.2847	-1.0844

Table 4. Values of a, b, c and corresponding standard deviation for TM 1 ternary liquid mixture at 308.15K.

Parameters	**A**	**b**	**c**	**σ**
$V^E x10^6/m^3mol^{-1}$	-921.044	-11310.3	-11987.2	0.3299
$\Delta K_s /TPa^{-1}$	47.2244	62.3324	2520.54	0.0454
$\Delta\eta /cP$	1.1080	36.3825	359.618	0.0008
ΔL_F x 10^{-10} /m	-74.064	57.21	-303.41	1.2792
$\Delta\beta_T$ x $10^{-11} /kg^{-1}K^{-1}m^2s$	-13.500	15.548	-1108.6	0.0005
ΔV_F x $10^{-07} /m^3mol^{-1}$	-50.295	-117.34	-2.7000	0.0250

Table 5. Values of a, b, c and corresponding standard deviation for the ternary liquid mixtures of TM 2 at 308.15K.

Parameters	**A**	**b**	**c**	**σ**
$V^E x10^6/m^3mol^{-1}$	2.1405	-31.2506	1828.93	0.0010
$\Delta K_s /TPa^{-1}$	290.497	1735.11	-54175	0.7515
$\Delta\eta /cP$	-9.0419	-10.7226	1324.86	0.0025
ΔL_F x 10^{-10} /m	4176	6139.6	27713	2.6680
$\Delta\beta_T$ x $10^{-08} /kg^{-1}K^{-1}m^2s$	526.14	690.71	3616.5	1.8650
ΔV_F x $10^{-10} /m^3mol^{-1}$	231.91	638.35	126.07	2.1610

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