Excess Thermodynamic Properties and Ftir Spectroscopy of Aceton-Isopropanol Liquid Binary Mixture

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Abstract

Experimental investigation was done using different instruments for the testing the properties of density, surface tension and viscosity in the case of pure and mixture system at the normal temperature of 25 ^{o}C and 1 atm. Excess volume was found to exhibit negative value at a mole fraction of 0.5. The deviation in the surface tension and viscosity were found of a positive value at the mole fraction value of 0.5. The experimental excess properties were correlated using the Redlich-Kister (RK) equation and showed an accepted standard deviation. The intermolecular interaction between acetone and isopropanol was found of negligible effect and showed a weakness in the hydrogen bonding according to the FTIR spectra for the mixture of acetone and isopropanol which agreed with the positive values of excess molar volume. Moreover, the values of surface tension and viscosity deviations were found of negative values for all the mole fraction range studied.

Keywords: Acetone, Density, Isopropanol, Viscosity, Excess molar volume, FTIR analysis, Surface tension, molecular interaction.

الخلاصة :

تمت الدراسه العمليه باستخدام اجهزه مختلفه لاختبار خواص الكثافه والشد السطحي واللزوجه للمكونات النقيه للسائل المدروس وكذلك للسائل الثنائي التركيب من الاسيتون والايزوبروبانول عند درجة حرارة 25 درجه مئويه وضغط جوي مقداره 1 ضغط جوي. لقد وجد ان قيمة الحجم المولي هي قيمة سالبه عند الكسر المولي الذي مقداره 0,5. بينما تم ايجاد قيم الانحراف في الشد السطحي والانحراف في اللزوجه عند الكسر المولي 0,5 وكانت قيم موجبه. تم ربط الخواص العمليه الزائديه بعضها مع البعض الاخر باستخدام معادلة ردلج كيستر وقد كانت النتائج ذات انحراف معياري مقبول. بواسطة تحليل المطياف الضوئي فقد تبين ان الترابط الجزيئي الداخلي لمكونات السائل الثنائي التركيب (من الاسيتون والايزوبروبانول) مهمول التاثير وايضا من خلال تحليل المطياف الضوئي لهذا المزيج فقد تبين الضعف في الاواصر الهيدروجينيه وهذا يتفق مع الحجم المولي الزائد.من ناحية اخرى فان قيم الشد السطحي وقيم الانحرافات في الشد السطحي و اللزوجه هي قيم سالبه لجميع الكسور الموليه المدروسه.

الكلمات الافتتاحيه :- اسيتون، الكثافه ، الايزوبروبانول ، اللزوجه، الحجم المولي الزائد، تحليل المطياف الضوئي ، الترابط الجزيئي .

1. Introduction

Many of the industrial processes required plenty of information regarding the physicochemical properties of different types of liquid mixtures. The physicochemical properties like excess properties, intermolecular interactions are important factors affecting the molecular structure and led to the non-ideal deviation in the transport phenomena (fluid flow, mass and heat transfer) (Dubey *et.al.*, 2016; Chen *et.al.*, 2015; Krishna *et.al.*, 2015; George *et.al.*, 2002; Ali *et.al.*, 2002). Many researchers worked on the excess properties of different liquid non-aqueous mixtures (Rowlinson and Swinton, 2013; Nain, 2013; Nain, 2009; Nain, 2013; Nain, 2008; Nain, 2007; Nain, 2016; Walmsley, 1978; Mehta *et.al.*, 2005; García *et.al.*, 1997; Walmsley *et.al.*, 1976; Yang *et.al.*, 2003; Curme and Young, 1925; Mohammadi *et.al.*, 2008; Krishna *et.al.*, 2017; Guo *et.al.*, 2011). The importance of thermodynamic excess properties is not useful only for the design and transport phenomena and but also in the case of providing a suitable data as a basis for developing new predictive equations and correlations. Moreover, the experimental data of density for a binary mixture can be used to calculate the excess volume property and related to the intermolecular interaction (Zorebski and Dzida, 2007; Krishna *et.al.*, 2008; Mehta *et.al.*, 2008). Hidayani et al. were used the extract of UncariaGambirRoxbleaf as capping agent and bio reducer in the production of AgNPs by using the isopropanol solvent (Hidayani *et. al.*, 2017). Smail et al. had established an expectation that the acetone and all ketones can be used as a solvent for the LRPs monomers (hydrophobic, hydrophilic) which catalyzed by metal (Smail *et.al.*, 2017). From the above review, it is concluded that the acetone and isopropanol are important solvent and used in many industrial processes and there is a need for experimental thermodynamic data which provide a pillar stone for the theoretical and design purposes. The present study provides experimental and numerical data for the excess volume (V^E), surface tension deviation (δ_σ) and viscosity deviation ($\delta\mu$). The Redlich-Kister equation had been used for the correlation of the experimental data. FTIR analysis had been obtained and checked for the Isopropanol-Acetone binary liquid mixtures in order to interpret the excess and deviation property.

2. Experimental

2.1. Materials and method

Acetone and Isopropanol were obtained from Fisher Scientific, U.K. The binary samples were provided for the experimentation using the electronic weight balance by CPA-225D, Germany, and manufactured by Sartorius. The precision for the measured weight was ±0.01 mg. The densities, surface tensions and viscosities for the pure and binary system of Acetone-Isopropanol. Density was measured using a densometer (Anton bar, DSA5000M, Austria). The calibration for the densometer was done using degassed distilled water (ρ=997.076 kg.m^3 at 298.15 K). Ethanol was used for the cleaning the vibrating tube of the densometer. The surface tension of the pure and binary liquid Acetone-Isopropanol were tested using LY-1068 tensometer, China. The precision of the instrument within the range of ± 0.0001. Ubbelohde capillary viscometer was used for the determination of the viscosity for the pure and binary system of Acetone-Isopropanol. The calibration method for the viscometer was done using distilled water and ethanol. Uncertinity of the instrument was estimated within the value of ±0.028 m^2.s^{-1}. FTIR spectra of the binary system of Acetone-Isopropanol was recorded using Bruker, Tensor II, Germany. The resolution of the instrument was within 1 cm^{-1} for the range of spectra between 4000-400 cm^{-1}.

3. Results and discussion

3.1. Density and excess molar volume

The densities of the pure and mixture of Acetone-isopropanol were measured experimentally and provided in the table 1 and table 2. The measured density was obtained at a temperature of 25^{o}C at normal pressure. Excess volume was calculated according to the following equation and put in the table 2:

$$V^E = V_m - \sum_{j=1}^{2} x_i\, V_i \cdots (1)$$

Where (V_m) can be calculated from the experimental values of the density for the mixture according to the equation (2).

$$V_m = \frac{[\sum_{i=1}^{2} x_i\,(M_{wi})]}{\rho} \cdots (2)$$

In the above equation (V_m: mixture molar volume, Vi: acetone or isopropanol volume, M_w: molecular weight of the acetone or isopropanol, ρ: density of the mixture volume, x_i: mole fraction of the acetone).

Figure 1 shows the variation of excess molar volume with the mole fraction of acetone. A nonlinear increase was observed in the excess molar volume with the increasing of acetone mole fractions. The non-ideal behavior of the excess molar volume can be returned to the intermolecular and intramolecular interactions in the binary system of acetone-isopropanol liquid mixture as stated by another researcher (Gnanakumari *et.al.*, 2007). A positive value in the excess molar volume was obtained for all mole fraction values and the maximum value of excess volume was obtained at the mole fraction value of 0.5.

Table 1 Experimental data of density (ρ), surface tension (σ) and viscosity (μ) for the pure chemical substances in the present study at 25 °C.

No.	Substance	M.wt (g/mol)	ρ (g/cm3)	σ (Dyn/cm)	μ (cp)
1	Acetone	58.08	0.784	23.7	0.32
2	Isopropanol	60.096	0.785	20.93	2.038

Table 2 Mixture density (ρ_m), excess volume (V^E), surface tension (σ), surface tension deviation (δ_σ), viscosity (μ_{mix}), viscosity deviation (δμ) for the samples of Acetone-Isopropanol mixture at (T=25°C and P=1 atm).

X_1	X_2	ρ_m	V^E	σ	δ_σ	μ_{mix}	δ_μ
0.1	0.9	0.786	-0.2	21.567	0.36	1.966	0.1
0.2	0.8	0.789	-0.41	22.134	0.65	1.934	0.24
0.3	0.7	0.791	-0.68	22.641	0.88	1.882	0.36
0.4	0.6	0.793	-0.85	23.078	1.04	1.790	0.44
0.5	0.5	0.7938	-0.89	23.415	1.1	1.659	0.48
0.6	0.4	0.793	-0.86	23.672	1.08	1.437	0.43
0.7	0.3	0.791	-0.66	23.739	0.87	1.185	0.35
0.8	0.2	0.788	-0.4	23.576	0.43	0.893	0.23
0.9	0.1	0.786	-0.19	23.553	0.13	0.621	0.13
1	0	0.784	0	23.7	0	0.32	0

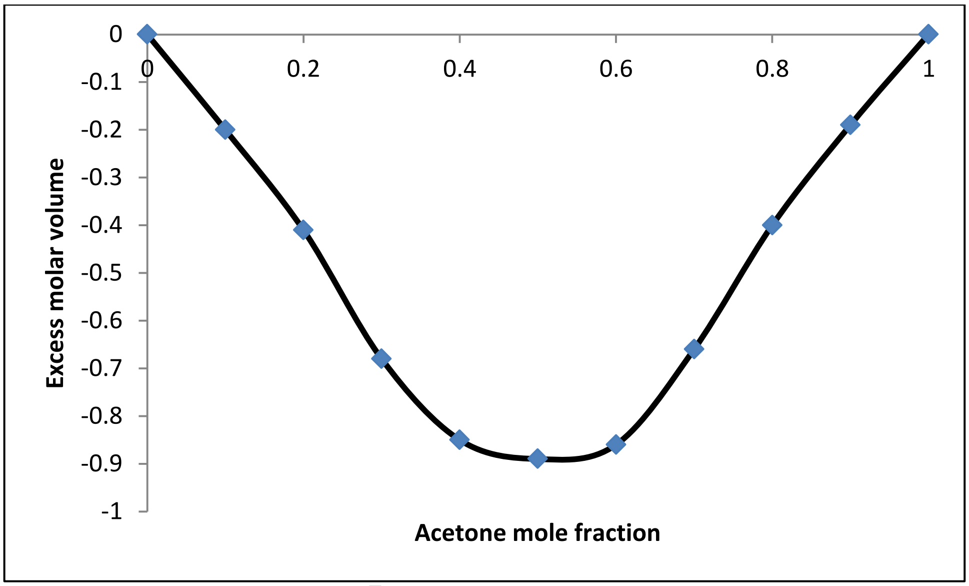


Fig. 1. Excess molar volume (V^E) as a function of the acetone mole fraction (X_1) for the Acetone-Isopropanol mixture at (T=25°C and P=1 atm).

3.2. Surface tension deviation

The surface tension deviation values were calculated from the experimental surface tension data according to the following equation (3):

$$\Delta\sigma = \sigma_m - (x_1\sigma_1 + x_2\sigma_2) \quad \dots (3)$$

The variation in the values of surface tension deviation (δ_σ) with the mole fraction of acetone was shown in the figure 2 and provided in the table 2. Obviously, a negative behavior in the surface tension deviation values was obtained at all the mole fraction values.

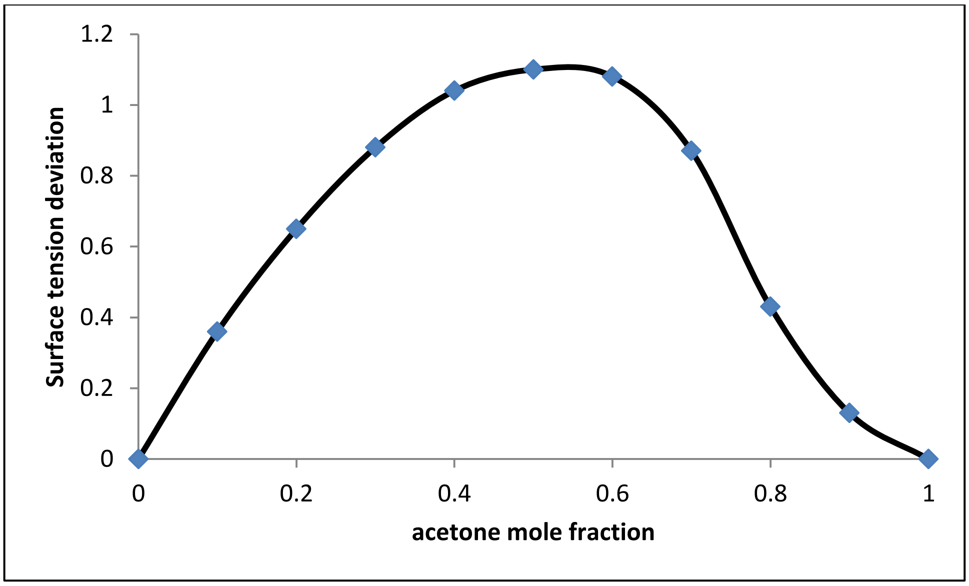


Fig. 2. Surface tension deviation (δ_σ) as a function of the acetone mole fraction (X_1) for the Acetone-Isopropanol mixture at ($T=25^oC$ and P=1 atm).

3.3. Viscosity deviation

Viscosity deviation was calculated from the experimental viscosity data of the pure and mixture binary liquid at different mole fraction at the following equation (4):

$$\Delta\eta = \eta_m - (x_1\,\eta_1 + x_2\eta_2) \cdots (4)$$

The resulted viscosity deviation data were provided in the table 2 and shown in figure 3. As in the case of surface tension deviation values, the values of viscosity deviation exhibited negative values. The maximum deviation in the viscosity was obtained at the mole fraction value of 0.5.

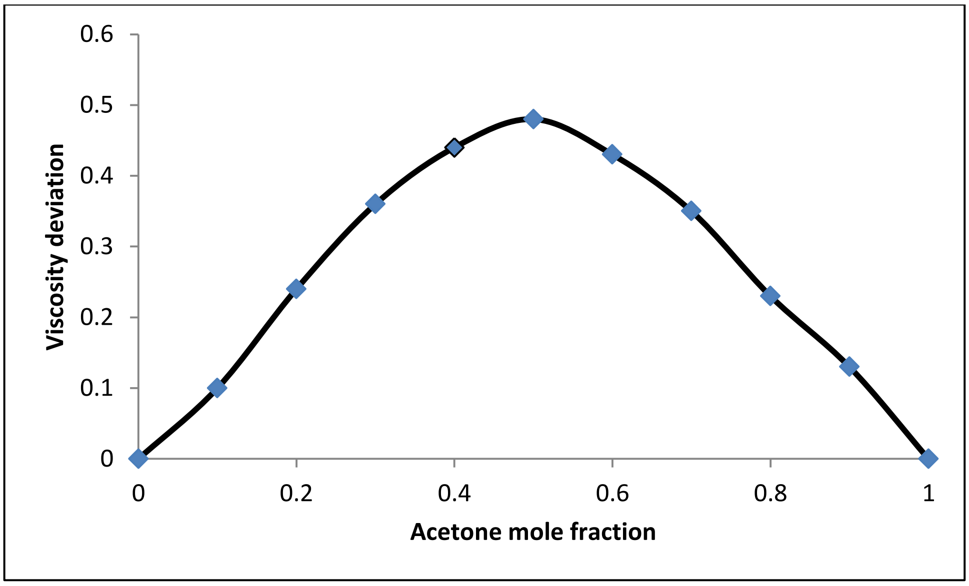


Fig. 3. Viscosity deviation (δ_η) as a function of the acetone mole fraction (X_1) for the Acetone-Isopropanol mixture at ($T=25^oC$ and P=1 atm).

3.4. Redlich-Kister correlation

The values of the excess molar volume, surface tension deviation and viscosity deviation were correlated to the Redlich-Kister equation of the following formula (Redlich and Kister, 1948):

$$V^{RE} = X_1 X_2 \sum_{i=0}^{2} A_i (X_1 - X_2)^i \cdots (5)$$

where X_1, X_2, are the mole fraction of Acetone and Isopropanol, A_i are the coefficients of the Redlich-Kister equation and provided in the table 3. The standard deviation (SD) for the binary system was calculated according to the following equation (6) and provided in the table 3.

$$SD = \left(\frac{\sum_{i=1}^{M} \left(F_{exp}^{E} - F_{cal}^{E} \right)^2}{M - N} \right)^{1/2} \cdots (6)$$

M, N are the experimental samples and constraints number, respectively.

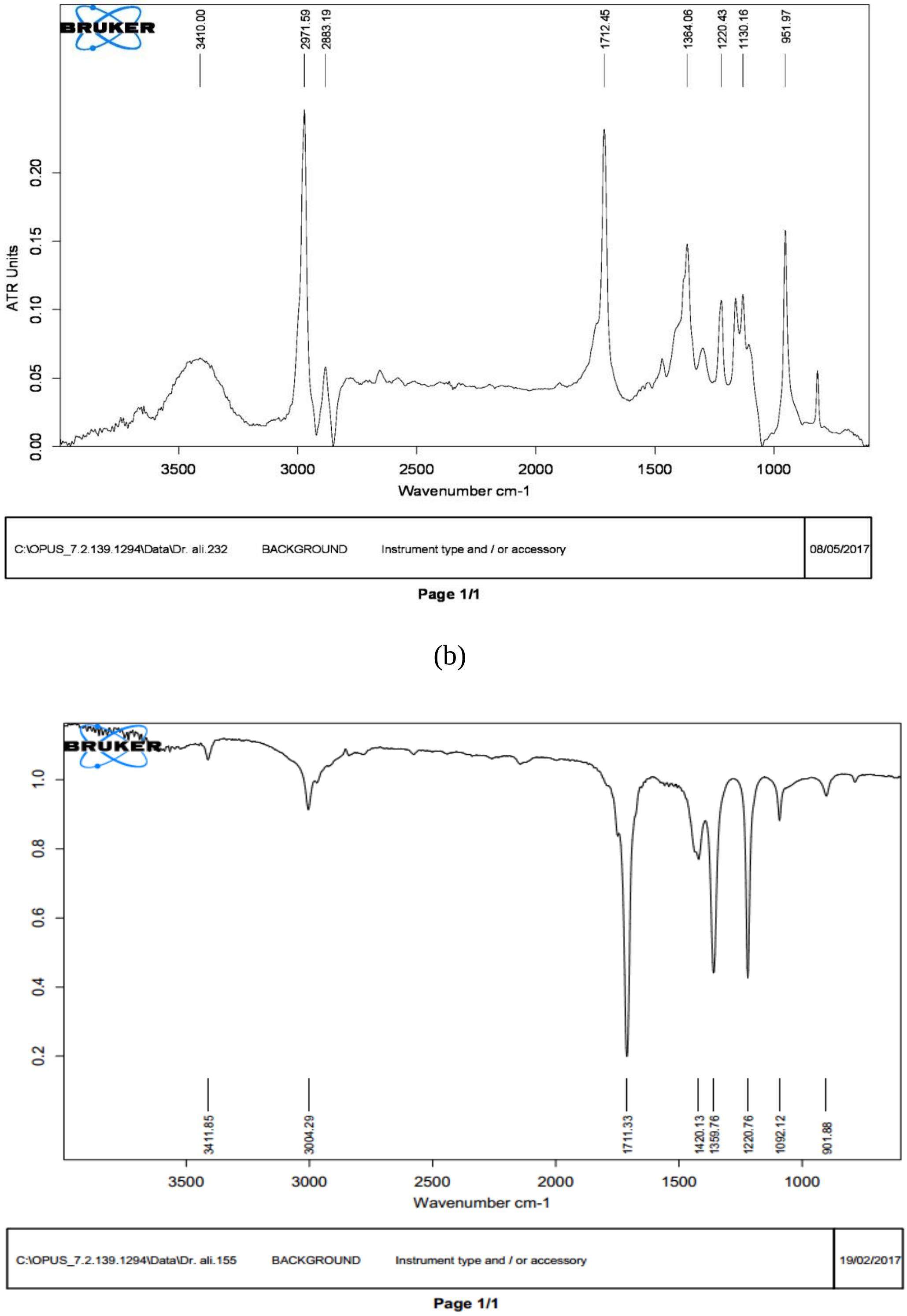
The experimental data showed an accepted deviation from the theoretical values as shown in the table 3.

Table 3 The coefficients of Redlich–Kister equation in the case of correlation the excess molar volume (V^E), surface tension deviation (δ_σ) and viscosity deviation of the samples of Acetone-Isopropanol mixture at (T=25°C and P=1 atm).

Function	Temperature, °C	a_0	a_1	a_2	a_3	a_4	SD
V^E	25 °C	-0.0055	- 0.9958	-9.493	21.096	-10.606	0.0003
δ_σ	25 °C	0.0294	2.1773	8.0119	-21.641	11.393	0.00002
δ_μ	25 °C	-0.0036	0.8572	3.2992	-8.3702	4.2249	0.0005

3.4. FTIR and intermolecular interaction

FTIR spectroscopy is an efficient instrument analysis tool for the characterization of polar chemical substances and can be used for the reorganization the functional group and the molecular interaction (Wei *et.al.*, 2013). For the acetone-isopropanol mixture, the FTIR spectra was shown in the figure 4. The spectra for the mixture of acetone-isopropanol at different mole fractions showed a very important behavior for the hydrogen bonding and explain the non-ideal behavior and the deviation in the thermodynamic properties as stated in the previous sections. As seen in the FTIR spectra, the broadening in the peak of the hydrogen referred to the intermolecular interaction effect and the sharpening explained as the intramolecular interaction effect. For the pure isopropanol, the spectra shows a broad O-H stretch at 2900 cm^{-1} while the most important peak in the pure acetone showed a strong C=O peak at 1715 cm^{-1}. While, for the mixture of acetone –isopropanol system, the increase in the mole fraction caused a slight shift in the place of the C=O peak to a higher wave number. The hydrogen bonding effect was found weak for the present mixture and led to the weakness in the intermolecular interaction between acetone and isopropanol. The result of the FTIR spectra agree with the result of excess volume and the conclusions stated by other researches (Hasan *et.al.*, 2011).



(b)

(a)

Fig. 5. FTIR Spectra of (a) pure Acetone, (b) DBSA-Acetone mixture of at Temperature=25^{o}C and Pressure=1 atm.

4. Conclusions

The experimental results for the excess volume, surface tension deviation and viscosity deviation showed non ideal behavior in the with the mole fraction variation. The correlation of the excess properties using the Redlich-Kister (RK) equation showed accepted deviation from the experimental data. The result of the FTIR showed an agreement to the result of the excess volume and proved that the intermolecular hydrogen bonding between acetone and isopropanol was weak for the mixture and can be concluded from the slight shift in the place of the C=O peak to a higher wave number.

References

Ali A., Nain A. K., Chand D., & Ahmad R. , 2006 , Volumetric and ultrasonic studies of molecular interactions in binary mixtures of dimethyl sulfoxide with some aromatic hydrocarbons at different temperatures. *Bulletin of the Chemical Society of Japan*, *79*(5), 702-710.

Chen F., Yang Z., Chen Z., Hu J., Chen C., & Cai J. , 2015 . Density, viscosity, speed of sound, excess property and bulk modulus of binary mixtures of γ-butyrolactone with acetonitrile, dimethyl carbonate, and tetrahydrofuran at temperatures (293.15 to 333.15) K. *Journal of Molecular Liquids*, *209*, 683-692..

Curme Jr G. O., & Young C. O. , 1925 . Ethylene Glycol. *Industrial & Engineering Chemistry*, *17*(11), 1117-1120.

Dubey G. P., Rani S., & Kaur P. , 2016, Study of molecular interactions in binary liquid mixtures containing tri-n-butylamine with 2-pentanone, 3-pentanone, and 4-methyl-2-pentanone: A thermophysical approach. *Journal of Molecular Liquids*, *222*, 415-424.

García B., Alcalde R., Leal J. M., & Matos J. S. , 1997 . Solute− solvent interactions in amide− water mixed solvents. *The Journal of Physical Chemistry B*, *101*(40), 7991-7997.

Gnanakumari P., Venkatesu P., Mohan K. R., Rao M. P., & Prasad D. H. L. , 2007 . Excess volumes and excess enthalpies of N-methyl-2-pyrrolidone with branched alcohols. *Fluid phase equilibria*, 252(1), 137-142.

Guo A., Hu X., Fang G., Shao S., & Zhang H. , 2011 . Enthalpies of dilution of 1, 3-propanediol and isomers of 2, 3-butanediol in dimethylsulfoxide+ water mixtures at 298.15 K. *Journal of Chemical & Engineering Data*, *56*(5), 2489-2500.

Hasan M., Hiray A. P., Kadam U. B., Shirude D. F., Kurhe K. J., & Sawant A. B. , 2011 . Densities, viscosities, speeds of sound, FT-IR and 1H-NMR studies of binary mixtures of n-butyl acetate with ethanol, propan-1-ol, butan-1-ol and pentan-1-ol at 298.15, 303.15, 308.15 and 313.15 K. *Journal of solution chemistry*, 40(3), 415-429. George, J., Sastry, N. V., Patel, S. R., & Valand, M. K. (2002). Densities, viscosities, speeds of sound, and relative permittivities for methyl acrylate+ 1-alcohols (C1− C6) at T=(308.15 and 318.15) K. *Journal of Chemical & Engineering Data*, *47*(2), 262-269.

Hidayani P., Aferta L., Ban T., & Ohya Y. , 2017 . Green Chemistry Formation of Stable Ag Nanoparticles (AgNPs) In Isopropanol Solvent. *Oriental Journal of Chemistry*, *33*(1), 87-91.

Krishna T. S., Nain A. K., Chentilnath S., Punyaseshudu D., & Munibhadrayya B. , 2016 . Densities, ultrasonic speeds, refractive indices, excess and partial molar properties of binary mixtures of imidazolium based ionic liquid with pyrrolidin-2-one at temperatures from 298.15 L to 323.15 K. *The Journal of Chemical Thermodynamics*, *101*, 103-114.

Krishna T. S., Nain A. K., Narendra K., Chenthilnath S., & Punyaseshudu D. , 2017 . Densities, ultrasonic speeds, excess and partial molar properties of binary mixtures of 2-pyrrolidone with isomeric propanediols at temperatures from 303.15 K to 323.15 K. *The Journal of Chemical Thermodynamics*, *111*, 129-141.

Krishna T. S., Sankar M. G., Raju K. T. S., Rao S. G., & Munibhadrayya B. , 2015 . Acoustic, volumetric, and optic study of binary mixture of 1-butyl-3-methylimidazoliumtetrafluoroborate with propylene glycols at T=(298.15 to 323.15) K. *Journal of Molecular Liquids*, *206*, 350-358.

Mehta S. K., Ram G., & Bhasin K. K. , 2005 . Effect of placement of hydroxyl groups in isomeric butanediol on the behaviour of thermophysical and spectroscopic properties of pyrrolidin-2-one. *The Journal of Chemical Thermodynamics*, *37*(8), 791-801.

Mehta S. K., Ram G., & Bhasin K. K. , 2008 . Molecular interactions of α, ω-alkanediols in pyrrolidin-2-one: Thermophysical and spectroscopic measurements. *The Journal of Chemical Thermodynamics*, *40*(3), 498-508.

Mohammadi A. H., Afzal W., & Richon D. , 2008 . Experimental data and predictions of dissociation conditions for ethane and propane simple hydrates in the presence of methanol, ethylene glycol, and triethylene glycol aqueous solutions. *Journal of Chemical & Engineering Data*, *53*(3), 683-686.

Nain A. K. , 2007, Densities and volumetric properties of (formamide+ ethanol, or 1-propanol, or 1, 2-ethanediol, or 1, 2-propanediol) mixtures at temperatures between 293.15 K and 318.15 K. *The Journal of Chemical Thermodynamics*, *39*(3), 462-473.

Nain A. K. , 2008 . Molecular interactions in binary mixtures of formamide with 1-butanol, 2-butanol, 1, 3-butanediol and 1, 4-butanediol at different temperatures: An ultrasonic and viscometric study. *Fluid Phase Equilibria*, *265*(1), 46-56.

Nain A. K. , 2013 . Densities, ultrasonic speeds, viscosities and excess properties of binary mixtures of methyl methacrylate with N, N-dimethylformamide and N, N-dimethylacetamide at different temperatures. *The Journal of Chemical Thermodynamics*, *60*, 105-116.

Nain A. K. , 2013 . Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C 4 to C 10) at temperatures from (288.15 to 318.15) K. *The Journal of Chemical Thermodynamics*, *59*, 49-64.

Nain, A. K. (2016). Densities and volumetric properties of (acetonitrile+ alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K. *The Journal of Chemical Thermodynamics*, *103*, 316-324.

Nain A. K., Srivastava T., Pandey J. D., & Gopal S. , 2009 . Densities, ultrasonic speeds and excess properties of binary mixtures of methyl acrylate with 1-butanol, or 2-butanol, or 2-methyl-1-propanol, or 2-methyl-2-propanol at temperatures from 288.15 to 318.15 K. *Journal of Molecular Liquids*, *149*(1), 9-17.

Redlich O., & Kister A. T. , 1948 . Algebraic representation of thermodynamic properties and the classification of solutions. *Industrial & Engineering Chemistry*, 40(2), 345-348.

Rowlinson J. S., & Swinton F. , 2013 . *Liquids and liquid mixtures: Butterworths monographs in chemistry*. Butterworth-Heinemann.

Smail R. B., Jezorek R. L., Lejnieks J., Enayati M., Grama S., Monteiro M. J., & Percec V. , 2017 . Acetone–water biphasic mixtures as solvents for ultrafast SET-LRP of hydrophobic acrylates. *Polymer Chemistry*, *8*(20), 3102-3123.

Walmsley, J. A. (1978). Self-association of 2-pyrrolidinone. 2. Spectral and dielectric polarization studies of benzene solutions. *The Journal of Physical Chemistry*, *82*(18), 2031-2035.

Walmsley, J. A., Jacob, E. J., & Thompson, H. B. (1976). An investigation of the self-association of 2-pyrrolidinone in cyclohexane and carbon tetrachloride by means of spectroscopic and dielectric polarization measurements. *The Journal of Physical Chemistry*, *80*(25), 2745-2753.

Wei, Q., Guo, X., Wang, Y., & Yang, H. (2013). Temperature-dependent FTIR study on three kinds of hydrogen-bonded benzoic acid dimers in their melt states. *Journal of Molecular Liquids*, 177, 225-228.

Yang, C., Ma, P., Jing, F., & Tang, D. (2003). Excess molar volumes, viscosities, and heat capacities for the mixtures of ethylene glycol+ water from 273.15 K to 353.15 K. *Journal of Chemical & Engineering Data*, *48*(4), 836-840.

Zorebski, E., & Dzida, M. (2007). Study of the acoustic and thermodynamic properties of 1, 2-and 1, 3-butanediol by means of high-pressure speed of sound measurements at temperatures from (293 to 318) K and pressures up to 101 MPa. *Journal of Chemical & Engineering Data*, *52*(3), 1010-1017.