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# MOLECULAR INTERACTIONSSTUDY IN BINARY SOLUTIONS OF ISOPROPYL ACETATE AND ISOPROPANOL AT 305,310,315 AND 320K TEMPERATURES

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## ABSTRACT

An investigation on molecular interaction is carried out from the measurements of density and viscosity of binary solutions of isopropyl acetate (1) and isopropanol (2) over the entire mole fraction from 0.1 to 1.0 at different temperatures (305,310,315 and 320K). Excess molar volume and deviation in viscosity are evaluated utilizing measured density and viscosity of systems studied. Positive values of excess molar volume obtained revealsrupturing of hydrogen bond of alcohol aggregates.Dispersion interaction leads to negative deviation in viscosity. Experimental values are correlated with theoretical values through Redlich-Kister polynomial equation. By the fitting of $V_m^E$and $\Delta\eta$, correlation parameters and standard deviation is calculated to explain correctness of results. Analysis of results of excess properties is used to predict the type and nature of possible molecular interactions.

***Key words:*** *Binary solution, Densities, molecular interaction, viscosity, Redlich-Kister.*

## I. INTRODUCTION

In recent time, thermodynamic properties of organic liquid mixtures are the requirement of chemists and researches. Estimation of these properties are appropriately immersed to considerate the nature of molecular interaction in liquid solutions. Knowledge of these properties of liquid mixtures helps in study of bio-molecular system[1], fragrance industry [2], production of bio-fuel[3], chemical engineering operation[4] etc.When two pure liquids are mixed their properties vary from its ideal behavior. Change in thermodynamic properties[5]from ideal pattern not only based on specific interaction taking place between solute-solvent molecules but structural changes also involved in constituent molecules.The main goal of study is explain molecular interaction by calculating excess properties and correlation equation.

Knowledge of volumetric and viscometric properties of liquid mixture is useful for desired purposes. Present study focused on study of molecular interaction in isopropyl acetate (1) and isopropanol (2). It is based on measurement of density and viscosity[6] directly from the liquid mixtures. From these data excess parameters[7] calculated and fitted in polynomial equation to validate correctness of experimental results. Excess quantities are used to explain molecular interaction [8]in binary system.

## II. METHOD AND MATERIAL

**Method:**Weighing measurements were performed on GC-103 electronic balance with $10^{-4}$ accuracy. Density measrmetns were done through Pycnometer. Viscosity of liquids determined using Ostwald's Viscometer. Flow time of liquid is noted using digital watch. Binary solution of different mole fraction from 0.1 to 1.0 were made and placed in dry place. For maintaining temperature thermostat is used. All the measurement is done the day of sample preparation. Measurements were performed three times and average values listed in table to consider as final values.

**Material:**Isopropyl acetate and isopropanol used in the present work were supplied by Loba Company. Chemicals were used without further purification and kept in desiccators. Purity of both the chemicals is 99%.

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## III. RESULT AND DISCUSSION

**Density-**Result of density measurements for binary solutions of isopropyl acetate (1) and isopropanol (2) is listed in Table 1 and plotted in Fig:1.

*Table-1. Densities of binary solution of isopropyl acetate (1) and isopropanol(2)*

| Mole fraction | Densities of binary (in gm/cm$^3$) | | | |
|---|---|---|---|---|
| x1 | 305 K | 310 K | 315 K | 320 K |
| 0 | 0.7806 | 0.7768 | 0.7724 | 0.7692 |
| 0.1 | 0.7882 | 0.7826 | 0.7773 | 0.7726 |
| 0.2 | 0.7954 | 0.7896 | 0.7837 | 0.7788 |
| 0.3 | 0.8029 | 0.7967 | 0.7909 | 0.7857 |
| 0.4 | 0.8107 | 0.8042 | 0.7984 | 0.7931 |
| 0.5 | 0.8189 | 0.8122 | 0.8064 | 0.8011 |
| 0.6 | 0.8280 | 0.8214 | 0.8159 | 0.8102 |
| 0.7 | 0.8381 | 0.8311 | 0.8256 | 0.8195 |
| 0.8 | 0.8472 | 0.8400 | 0.8349 | 0.8289 |
| 0.9 | 0.8550 | 0.8481 | 0.8434 | 0.8378 |
| 1 | 0.8613 | 0.8547 | 0.8504 | 0.8454 |

Density of binary solution, increase on increasing composition of ester [9]at same temperature and decreases with increasing temperatures at fixed mole fraction.

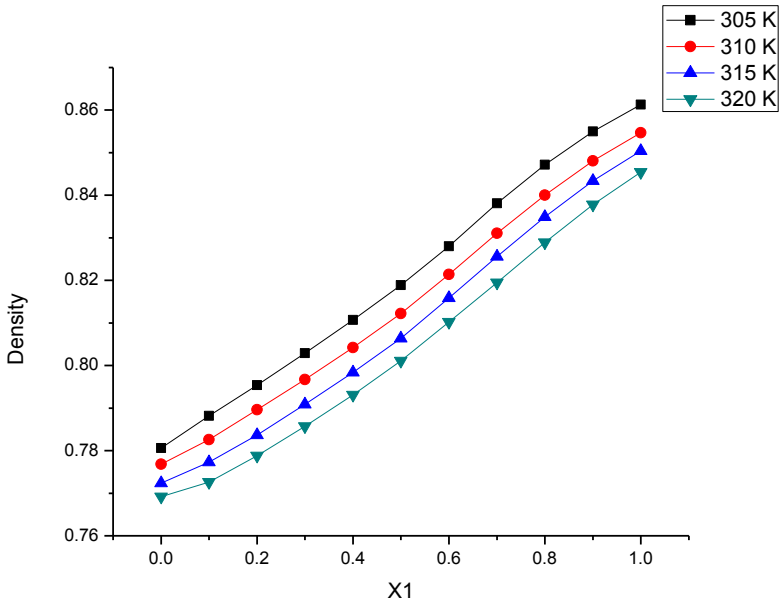


*Fig: 1 Plot of X1 v/s Density for Binary solution of isopropyl acetate (1) and isopropanol (2)*

**Excess Molar Volume-** From the experimental density data excess molar volume of binary solutions are calculated using following equation and given in Table 2.

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$$VmE = \frac{X1M1 + X2M2}{\rho_s} - \left(\frac{X1M1}{\rho1} + \frac{X2M2}{\rho2}\right) \ldots\ldots\ldots (1)$$

Where$\rho_S$ is density of binary solution; X1, M1, ρ1 and X2, M2, ρ2 are the mole fraction, molecular weight and density of pure compound 1 and 2 respectively.

*Table-2. Excess Molar Volume of binary solution of isopropyl acetate (1) and isopropanol (2)*

| Mole fraction | Excess molar of binary (in $cm^3$/mol ) | | | |
|---|---|---|---|---|
| X1 | 305 K | 310 K | 315 K | 320 K |
| 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 0.1 | 0.4372 | 0.5916 | 0.6817 | 0.8249 |
| 0.2 | 0.8186 | 0.9738 | 1.1382 | 1.2926 |
| 0.3 | 1.0922 | 1.2570 | 1.4292 | 1.6057 |
| 0.4 | 1.2513 | 1.4233 | 1.6075 | 1.7686 |
| 0.5 | 1.2766 | 1.4464 | 1.6359 | 1.7836 |
| 0.6 | 1.0996 | 1.2240 | 1.3831 | 1.5610 |
| 0.7 | 0.7120 | 0.8659 | 1.0254 | 1.2348 |
| 0.8 | 0.3739 | 0.5085 | 0.6241 | 0.7990 |
| 0.9 | 0.1140 | 0.1946 | 0.2401 | 0.3442 |
| 1 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

From the Fig: 2 it is observed that excess molar volume is positive[10] over the entire composition and temperature range. Excess molar volumeincreasewith addition of ester attained maximumup to X1 = 0.5, than decreases on addition of ester. Positive excess molar volume is due to rupturingof hydrogen bond of isopropanol moleculesthus breaking of aggregates gives increases volume. Excess molar volume increases[11] on increasing temperatures.

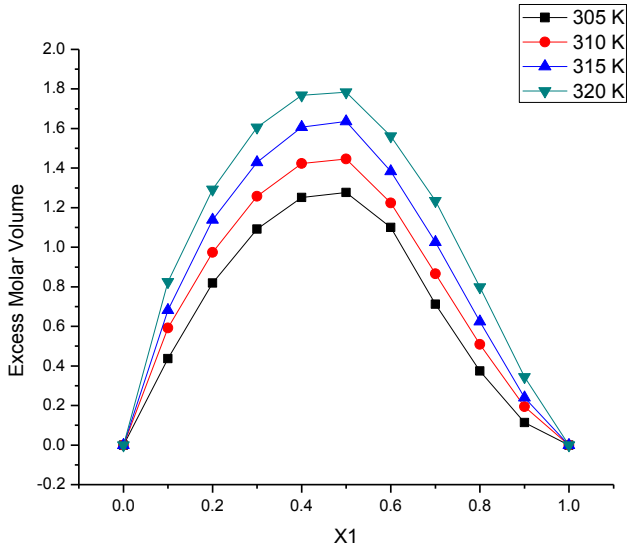


*Fig: 2 Plot of X1 v/s Excess Molar Volume for Binary solution of isopropyl acetate (1) and isopropanol (2)*

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**Viscosity** –Viscosity of binary solutions of isopropyl acetate (1) and isopropanol (2) listed in Table 3 and graph is shown in Fig:3.

*Table-3. Viscosity of binary solution of isopropyl acetate (1) and isopropanol(2)*

| Mole Fraction | viscosities of binary η(m.Pa.s) | | | |
|---|---|---|---|---|
| X1 | 305 K | 310 K | 315 K | 320 K |
| 0 | 1.7312 | 1.6655 | 1.5713 | 1.4730 |
| 0.1 | 1.5487 | 1.4985 | 1.4239 | 1.3414 |
| 0.2 | 1.3839 | 1.3374 | 1.2682 | 1.1943 |
| 0.3 | 1.2296 | 1.1866 | 1.1245 | 1.0579 |
| 0.4 | 1.0855 | 1.0463 | 0.9909 | 0.9314 |
| 0.5 | 0.9491 | 0.9138 | 0.8614 | 0.8090 |
| 0.6 | 0.8246 | 0.7932 | 0.7499 | 0.7030 |
| 0.7 | 0.7154 | 0.6869 | 0.6485 | 0.6068 |
| 0.8 | 0.6168 | 0.5912 | 0.5574 | 0.5208 |
| 0.9 | 0.5295 | 0.5108 | 0.4770 | 0.4462 |
| 1 | 0.4613 | 0.4350 | 0.3941 | 0.3604 |

Viscosity of solution decrease [12]with increasing temperatures and again observed that decreasing pattern with addition of ester in solution.

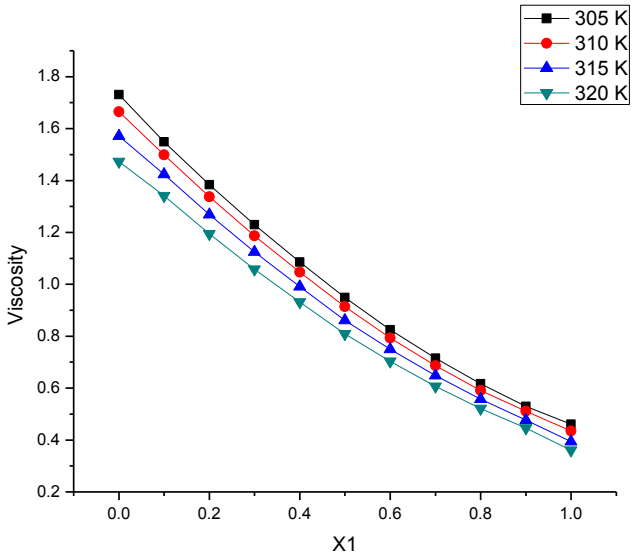


***Fig: 3 Plot of X1 v/s Viscosity for Binary solution of isopropyl acetate (1) and isopropanol (2)***

**Deviation in Viscosity**

Equation 2 is used to evaluate deviation in viscosity of binary solution which is presented in Table 4 and plot of X1 v/s Δη in Fig:4.

$$\Delta\eta = \eta_s - (X1\eta1 + X2\eta2) \dots\dots\dots\dots (2)$$

Where $\eta_S$is viscosity of binary solution; X1, $\eta_1$ and X2, $\eta_2$ are the mole fraction and viscosities of pure component 1 and 2 respectively.

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*Table-4. Deviation in Viscosity of binary solution of isopropyl acetate (1) and isopropanol(2)*

| Mole fraction | Deviation in Viscosity | | | |
|---|---|---|---|---|
| X 1 | 305 K | 310 K | 315 K | 320 K |
| 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 0.1 | -0.0555 | -0.0440 | -0.0297 | -0.0203 |
| 0.2 | -0.0933 | -0.0820 | -0.0677 | -0.0562 |
| 0.3 | -0.1206 | -0.1098 | -0.0937 | -0.0814 |
| 0.4 | -0.1378 | -0.1270 | -0.1096 | -0.0965 |
| 0.5 | -0.1472 | -0.1364 | -0.1213 | -0.1078 |
| 0.6 | -0.1447 | -0.1340 | -0.1151 | -0.1024 |
| 0.7 | -0.1269 | -0.1173 | -0.0988 | -0.0874 |
| 0.8 | -0.0985 | -0.0900 | -0.0721 | -0.0621 |
| 0.9 | -0.0588 | -0.0473 | -0.0348 | -0.0255 |
| 1 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

Deviation in viscosity found negative[13]for binary solution of isopropyl acetate and isopropanol in all over mole fraction and temperatures. Negative values are due to dispersion forces[14] in solution. Breaking of dipolar attraction of isopropanol is also ascribable to negative deviation in viscosity.

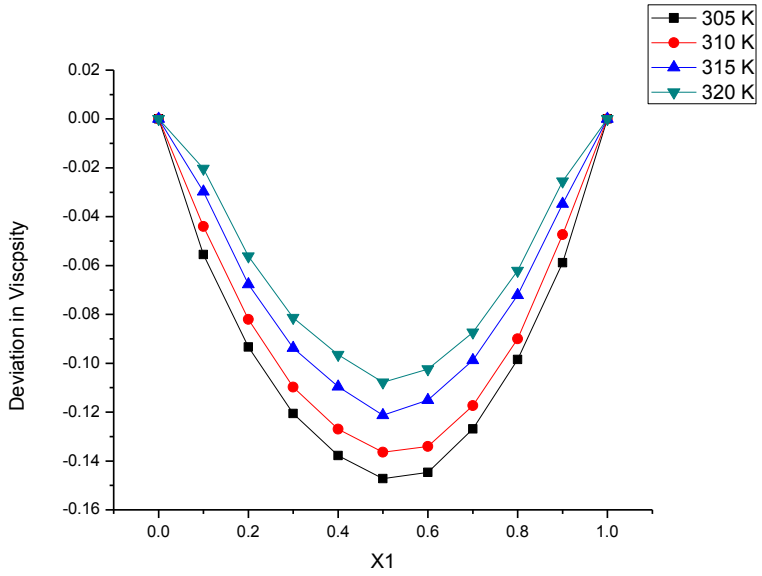


***Fig: 4 Plot of X1 v/s Deviation in viscosity for Binary solution of isopropyl acetate (1) and isopropanol (2)***

**Redlich- Kister Equation-**

Excess properties were fitted in Redlich-Kister[15] polynomial equation (3) and used to correlate experimental results

$$Y = X1.X2\sum_{i=0}^{n} A_i(X1 - X2)^i \dots\dots\dots\dots (3)$$

Where Y is excess molar volume or deviation in viscosity, X1 and X2 are mole fractions of component 1 and 2 respectively. $A_i$ is correlation parameters [16]obtained by fitting[17]of experimental result. The magnitude of correlation is evaluated by calculating standard deviation using following equation (4). Correlationparametersand standard deviation is given in Table 5.

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$$\sigma = \sqrt{\frac{\Sigma\,(Y_{exp} - Y_{cal})^2}{(N - m)}} \ldots\ldots\ldots(4)$$

Where σ stands for standard deviation, N are number of data point, m is number of correlation parameters.

***Table-5. Correlation parameters and Standard deviation for Redlich- Kister equation for binary solution of isopropyl acetate (1) and isopropanol(2) at 305,310,315 and 320K.***

| | T/K | A0 | A1 | A2 | A3 | A4 | σ |
|---|---|---|---|---|---|---|---|
| $V_m^E$ | **305** | 4.961 | 0.998 | -0.991 | 2.599 | -3.7601 | 0.08264 |
| | **310** | 5.681 | 0.889 | -0.995 | 2.478 | -3.0212 | 0.09546 |
| | **315** | 6.401 | 1.391 | -0.997 | 2.882 | -2.152 | 0.06664 |
| | **320** | 7.194 | 1.603 | -0.998 | 2.745 | -2.178 | 0.06073 |
| Δη | **305** | -0.602 | 0.011 | 0.015 | 0.201 | 0.0223 | 0.00703 |
| | **310** | -0.551 | 0.014 | 0.016 | 0.135 | 0.0212 | 0.00422 |
| | **315** | -0.477 | 0.011 | 0.049 | 0.123 | 0.0201 | 0.00573 |
| | **320** | -0.432 | 0.058 | 0.105 | 0.015 | 0.0531 | 0.00597 |

## IV. CONCLUSION

Density and viscosity of binary solution of isopropyl acetate and isopropanol are reported in present investigation. Excess molar volume and deviation in viscosity evaluated from experimental values. Excess parameters are fitted in Redlich-Kister polynomial equation and good agreement is found. Positive excess molar volumes discuss in terms of breaking hydrogen bond of alcohol molecule in presence of ester. Negative deviation in viscosity is explained due to dispersion forces and breaking of dipole-dipole attraction of alcohol

## REFERENCES

[1] *T. Imai, "Molecular theory of partial molar volume and its applications to biomolecular systems," Condens. Matter Phys., vol. 10, no. 3, pp. 343–361, 2007.*
[2] *H. Djojoputro and S. Ismadji, "Density and viscosity correlation for several common fragrance and flavor esters," J. Chem. Eng. Data, vol. 50, no. 2, pp. 727–731, 2005.*
[3] *F. Karaosmanoğlu, K. B. Cığızoğlu, M. Tüter, and S. Ertekin, "Investigation of the Refining Step of Biodiesel Production," Energy & Fuels, vol. 10, no. 4, pp. 890–895, 1996.*
[4] *F. Ouaar, A. Negadi, I. Bahadur, and L. Negadi, "Thermophysical approach to understand the nature of molecular interactions and structural factor between methyl isobutyl ketone and organic solvents mixtures," J. Chem. Thermodyn., vol. 113, pp. 291–300, 2017.*
[5] *G. a. Krestov, "Modern aspects of thermodynamics and structure of nonaqueous solutions," Pure Appl. Chem., vol. 59, no. 9, pp. 1203–1214, 1987.*
[6] *R. J. Fort and W. R. Moore, "Viscosities of binary liquid mixtures," Trans. Faraday Soc., vol. 62, pp. 1112–1119, 1966.*
[7] *R. W. Missen, "Use of the term 'excess function,'" Ind. Eng. Chem. Fundam., vol. 8, no. 1, pp. 81–84, 1969.*
[8] *S. Manukonda, G. P. Kumar, and C. P. Babu, "Molecular Interactions in Binary Organic Liquid Mixtures Containing Ethyl Oleate and Ethanol at 2MHz Frequency," Int. Lett. Chem. Phys. Astron., vol. 40, pp. 17–23, 2014.*
[9] *P. S. Nikam, T. R. Mahale, M. Hasan, P. Chemistry, M. S. G. College, and M. Camp, "Density and Viscosity of Binary Mixtures of Ethyl Acetate with Methanol, Ethanol, Propan-1-ol, Propan-2-ol, Butan-1-ol, 2-Methylpropan-1-ol, and 2-Methylpropan-2-ol at (298.15, 303.15, and 308.15) K," J. Chem. Eng. Data, vol. 41, no. 5, pp. 1055–1058, 1996.*

ISSN 2348 – 8034
Impact Factor- 5.070

[10] *P. S. Nikam, T. R. Mahale, and M. Hasan, "Densities and viscosities for ethyl acetate + pentan-1-ol, + hexan-1-ol, + 3,5,5-trimethylhexan-1-ol, + heptan-1-ol, + octan-1-ol, and + decan-1-ol at (298.15, 303.15, and 308.15) K," J. Chem. Eng. Data, vol. 43, no. 3, pp. 436–440, 1998.*

[11] *H. Djojoputro and Suryadi Ismadji, "Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol , Ethanol , and 1-Propanol at ( 293 . 15 , 303 . 15 , and 313 . 15 ) K," J. Chem. Eng. Data, vol. 50, no. 4, pp. 1343–1347, 2005.*

[12] *S. S. Patil, S. R. Mirgane, and B. R. Arbad, "Excess molar volumes and deviation in viscosities of binary liquid mixtures of acrylic esters with hexane-1-ol at 303.15 and 313.15 K," J. Saudi Chem. Soc., vol. 18, pp. 945–952, 2014.*

[13] *X. Wang, X. Wang, and D. Wang, "Volumetric and viscometric properties of ethyl caprate + 1-propanol, + 1-butanol, and + 1-pentanol from 283.15 K to 318.15 K," J. Mol. Liq., vol. 225, pp. 311–319, 2017.*

[14] *N. V. Sastry and M. K. Valand, "Thermodynamics of acrylic ester-organic solvent mixtures. V. viscosities and excess viscosities of alkyl acrylates-1-alcohol binary mixtures at 298.15 and 308.15 K," Int. J. Thermophys., vol. 18, no. 6, pp. 1387–1403, 1997.*

[15] *O. Redlich and A. T. Kister, "Algebraic Representation of Thermodynamic Properties and the Classification of Solutions," Ind. Eng. Chem., vol. 40, no. 2, pp. 345–348, 1948.*

[16] *R. Belda, "A proposed equation of correlation for the study of thermodynamic properties (density, viscosity, surface tension and refractive index) of liquid binary mixtures," Fluid Phase Equilib., vol. 282, pp. 88–99, 2009.*

[17] *P. J. Flory, R. A. Orwoll, and A. Vrij, "Statistical Thermodynamics of Chain Molecule Liquids. I. An Equation of State for Normal Paraffin Hydrocarbons," J. Am. Chem. Soc., vol. 86, no. 17, pp. 3507–3514, 1964.*