JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

Density and Viscosity Study of Binary Solutions of n-amyl acetate(1) and isopropanol(2) at Various Temperatures

[1]Dr. Chanchala Joshi, [2]Dr. Geetha Sarasan, [3]Dr. Madhu Khandelwal, [4]Dr.Namrata Pathak

[1]Dept. of Chemistry, Govt. Bhagat Singh College Jaora,Ratlam M.P.

[2]Dept. of Chemistry, Govt Holkar Science College,Indore M.P

[3]Dept of Chemistry, Govt Nehru P.G. College, Agar Malwa M.P

[4]Dept. of Chemistry, Govt Holkar Science College,Indore M.P

Abstract: An investigation carried out from the measurement of density and viscosity of binary solutions of n- amyl acetate and isopropanol over the mole fraction range 0.1 to 1.0 at different temperatures (305,310,315 and 320 K). Excess molar volume and deviation in viscosity were calculated using densities and viscosities values. Positive values of excess molar volume and negative values of deviation in viscosity are obtained. To validate the result, excess quantities such as excess molar volume and deviation in viscosities are fitted in Redlich-Kister polynomial equation. Experimental viscosities are employed in various semi-empirical models to validate correctness of results. Experimental and calculated quantities are interpreted in terms of possible molecular interaction in binary solution.

Key words: Binary solution, Density, Viscosity, Molecular interaction, Redlich-Kister equation.

I. INTRODUCTION

Esters are alkyl derivatives of carboxylic acid having functional group alkyl alkanoate formed by reaction of carboxylic acids and alcohol. These are volatile organic compounds having specific odour. Esters can be obtained from natural compounds i.e. natural esters and synthetic esters can be prepared in laboratory for specific application. Alcohol is chief component of laboratory as well as industrial applications. In last decade study of ester in non-aqueous solutions were concerned due to industrial processes such as fragrance industries [1], chemical plants, production of bio-fuel [2], chemical engineering and pharmaceuticals [3]. When ester and alcohol are mixed their properties vary from their ideal behavior. Variation from ideal behavior leads to specific solute-solvent and solvent –solvent interaction in the binary systems. Additionally, the study includes the calculation of derived functions such as excess molar volume and deviation in viscosity which is useful to understand the nature and type of molecular interaction [4] between the components. The work is therefore aimed to evaluate the excess parameters and validate the results with the help of Redlich-Kister polynomial equation. Present work gives practical utility and predictable transport properties of systems involving binary solutions of esters [5].

II. MATERIAL AND EXPERIMENTAL METHOD

Material: n-amyl acetate and isopropanol used in our work are supplied by Loba company. Chemicals are used without further purification and kept in decicator. Purity of both the chemicals are 99%. **Experimental Method:** The weighing performed on electronic balance GC-103 with accuracy 0.0001kg. A pycnometer is used to measurement of density. Ostwald's vicometer is used to measure viscosities of binary solution and that of pure component. Thermostat is used to maintain temperature. Composition of binary solutions varies from 0.1 to 1.0 M and kept in air tight bottles. Measurement performed same day of sample preparation. All the measurements performed three times and taken average values as final value.

III. RESULT AND DISCUSSION

Density: Density values for binary systems of n-amyl acetate (1) and isopropanol (2) are given in table 1 and plotted in Fig 1. Density values are increases over the entire range of mole fraction and decreasing values are found on temperature increment in a fixed composition[6].

Table:1 Experimental Densities of binary solutions of n-amyl acetate (1) and isopropanol (2) at different temperatures.

n-amyl acetate(1) + isopropanol(2)				
Mole fraction	**Densities of binary (in gm/cm^3)**			
X_1	**305 K**	**310 K**	**315 K**	**320 K**
0	0.7806	0.7768	0.7724	0.7692
0.1	0.7920	0.7864	0.7803	0.7739
0.2	0.7999	0.7936	0.7875	0.7809
0.3	0.8068	0.8008	0.7945	0.7877
0.4	0.8145	0.8081	0.8018	0.7954
0.5	0.8227	0.8163	0.8100	0.8037
0.6	0.8317	0.8250	0.8194	0.8128
0.7	0.8409	0.8340	0.8287	0.8221
0.8	0.8495	0.8427	0.8376	0.8310
0.9	0.8578	0.8520	0.8469	0.8401
1	0.8653	0.8604	0.8568	0.8514

Fig 1 Plot of density v/s X_1(mole fraction of n-AA) at different temperatures.

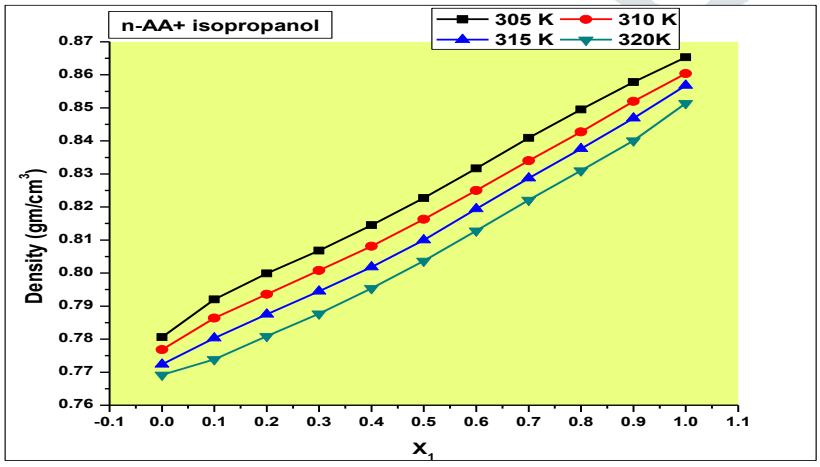

Fig 1 Plot of density v/s X_1(mole fraction of n-AA) at different temperatures.

Excess molar volume: Experimental density data utilized to evaluate excess molar volume using equation 1, which are shown in Table 2 and plotted in Fig 2 for the binary solutions of n-amyl acetate (1) and isopropanol(2).

$$V_m^E = \frac{X_1M_1 + X_2M_2}{\rho_{12}} - \left(\frac{X_1M_1}{\rho_1} + \frac{X_2M_2}{\rho_2}\right) \dots\dots\dots (1)$$

Where ρ_{12} is density of binary solutions; X_1, M_1, ρ_1 and X_2, M_2, ρ_2 are the mole fraction, molecular weight and density of pure compound 1 and 2 respectively.

Table: 2 Excess Molar Volume of binary solutions of n-AA acetate(1) and iso- propanol (2) at different temperature

n-amyl acetate(1) + isopropanol(2)				
Mole fraction	**Excess molar of binary (in cm^3/ mol)**			
X_1	**305 K**	**310 K**	**315 K**	**320 K**
0	0.0000	0.0000	0.0000	0.0000
0.1	0.3984	0.5795	0.7740	1.1027
0.2	0.9734	1.2450	1.4763	1.8260
0.3	1.5307	1.7656	2.0545	2.4272
0.4	1.8343	2.1194	2.4654	2.7632
0.5	1.9277	2.2198	2.5914	2.8737
0.6	1.7484	2.0875	2.3861	2.6848
0.7	1.3960	1.7651	2.0171	2.3090
0.8	0.9793	1.3410	1.5761	1.8546
0.9	0.4931	0.6575	0.9130	1.1928
1	0.0000	0.0000	0.0000	0.0000

Positive values of excess molar volume are obtained in all composition and temperature range, which shows that breaking of hydrogen bonding in ester molecules [7]. On increasing temperature positive values increases at fixed composition because high temperature [8]favors breaking of H- bonding in molecules of esters.

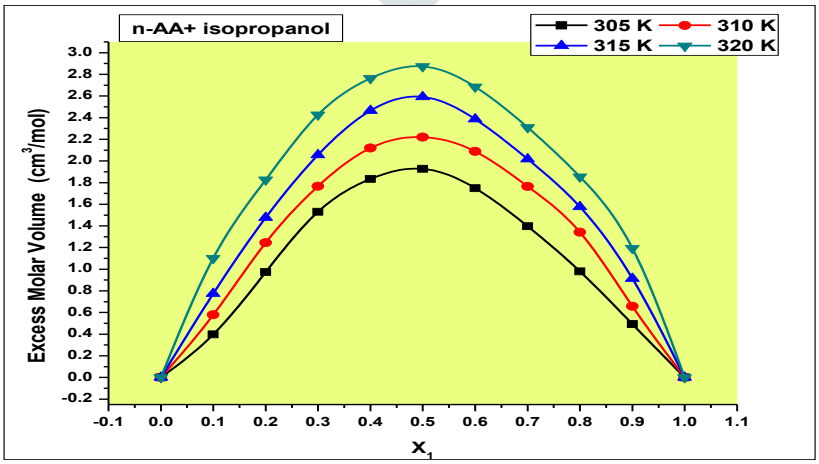

Fig 2: Plot of Excess Molar Volume v/s X_1(mole fraction of n-AA) at different temperatures.

Viscosity: Viscosity values are measured for binary solutions of n-amyl acetate (1)and isopropanol (2) are tabulated in (Table 3) and plotted in Fig 3. It is observed that values decrease over the entire range of mole fraction [9] and temperature also.

Table:3 Experimental Viscosity of Binary solutions of n-amyl acetate (1) and isopropanol (2) at 305, 310,315 and 320K.

n- amyl acetate(1) + iso propanol (2)				
	Viscosities of binary η(m.Pa.s)			
X_1	305 K	310 K	315 K	320 K
0	1.7312	1.6655	1.5713	1.4730
0.1	1.5642	1.5096	1.4270	1.3431
0.2	1.4259	1.3734	1.2991	1.2209
0.3	1.2963	1.2450	1.1721	1.1019
0.4	1.1758	1.1229	1.0580	0.9877
0.5	1.0671	1.0140	0.9543	0.8897
0.6	0.9668	0.9168	0.8637	0.8074
0.7	0.8768	0.8299	0.7786	0.7306
0.8	0.7920	0.7489	0.7079	0.6638
0.9	0.7236	0.6826	0.6473	0.6083
1	0.7103	0.6611	0.6212	0.5796

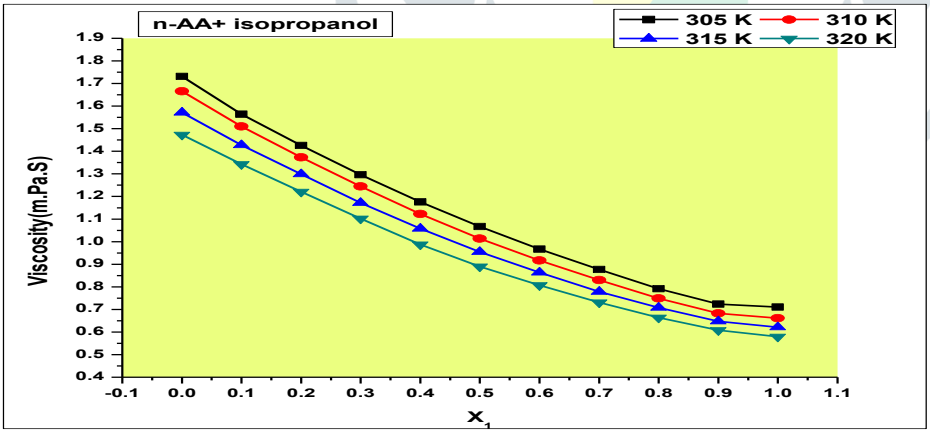

Fig 3: Plot of Viscosity v/s X_1 (mole fraction of n-amyl acetate) at different temperatures.

Deviation in viscosity: Deviation in viscosity is evaluated using equation no 2, result were evaluated and tabulated in Table no 4 and shown in Fig 4.

$$\Delta\eta_{12}\ (\mathbf{m.Pa.s}) = \eta_{12} - (\mathbf{X_1\eta_1 + X_2\eta_2}) \ldots\ldots (\mathbf{2})$$

Where η_{12} is viscosity of binary solutions of iso-pentyl acetate(1) and iso-propanol(2); X_1, η_1 and X_2, η_2 are the mole fraction and viscosities of pure component 1 and 2 respectively.

Table:4 Deviation in Viscosities of Binary solutions of n-amyl acetate (1) and isopropanol (2) at 305, 310,315 and 320K.

n-amyl acetate(1) + isopropanol (2)				
	Deviation in viscosities of binary Δη (m.Pa.s)			
X_1	305 K	310 K	315 K	320 K
0	0.0000	0.0000	0.0000	0.0000
0.1	-0.0649	-0.0554	-0.0493	-0.0406
0.2	-0.1011	-0.0912	-0.0822	-0.0735
0.3	-0.1287	-0.1192	-0.1142	-0.1031
0.4	-0.1471	-0.1408	-0.1333	-0.1279
0.5	-0.1536	-0.1493	-0.1419	-0.1366
0.6	-0.1519	-0.1460	-0.1375	-0.1295
0.7	-0.1398	-0.1325	-0.1277	-0.1170
0.8	-0.1225	-0.1131	-0.1033	-0.0944
0.9	-0.0889	-0.0790	-0.0689	-0.0606
1	0.0000	0.0000	0.0000	0.0000

Negative values of deviation are obtained [10] in all temperature and composition range. Negative values of deviation in viscosities shows that lowering in viscosity[11].

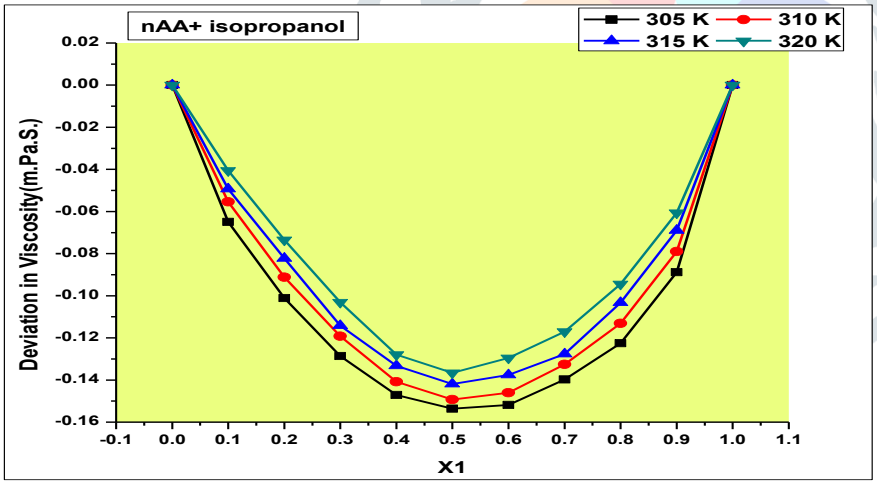

Fig 4: Plot of Deviation in Viscosity v/s X_1 (mole fraction of n-amyl acetate) at different temperatures.

Correlation of thermodynamic properties: Properties of binary solutions show non-linear behavior, which are explained using correlation equations. These equations are reliable tool to explain properties of binary solution. Extent of correlation used to evaluate physiochemical behaviour of binary liquid solutions.

Redlich-Kister Polynomial equation for Binary Systems

Redlich and Kister [12] suggested a polynomial equation [13] for the correlations of binary liquid mixtures. Derived parameters are fitted in this equation to evaluate magnitude of interaction in binary mixtures.

$$\Delta Y = X_1 X_2 \sum_{i=0}^{n} A_i (X_1 - X_2)^i \ldots\ldots (3)$$

Where A_i are the fitted parameters, empirically more the number of fitting parameter better of the fitting.

Standard Deviation (SD) : Standard deviation or standard errors are used to summarize numerical data and estimate population parameters [14] from sample. The magnitude of correlation is evaluated by calculating standard deviation using equation

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

Where S is standard deviation, N is number of data points in the experiment and m is number of fitting parameters. Minimum values of standard deviation support the more precise measurements.

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

Binary solution of n-AA(1) + Isopropanol (2)							
Excess parameters	**T/K**	**A_0**	**A_1**	**A_2**	**A_3**	**A_4**	**S**
V_m^E	305	7.6621	-0.589	-3.085	2.001	-2.014	**0.0906**
	310	8.8624	-0.789	-2.575	1.995	-1.954	**0.0754**
	315	9.999	-0.862	-1.212	0.995	-0.854	**0.0882**
	320	11.409	-0.094	-0.035	0.651	-0.0002	**0.0951**
$\Delta\eta$	305	-0.612	-0.021	-0.163	0.375	0.0295	**0.00888**
	310	-0.588	-0.019	-0.152	0.298	0.0289	**0.00538**
	315	-0.561	-0.017	-0.136	0.281	0.0276	**0.00446**
	320	-0.536	-0.013	-0.078	0.362	0.0262	**0.00598**

Semi-empirical models for viscosity

Experimental viscosity correlated in several semi-empirical model of viscosity such as Gurnberg-Nissan model[15], Hind model[16] and Tamura-Kurata model[17].

Gurnberg-Nissan model - In this model, the following equation is proposed to correlate experimental and theoretical viscosities

$$\ln \eta_{12} = X_1 \ln \eta_1 + X_2 \ln \eta_2 + X_1X_2G_{12} \text{…….(5)}$$

Hind model - Interaction of mixing component can also be estimated by Hind equation

$$\ln \eta_{12} = X_1 \ln \eta_1 + X_2 \ln \eta_2 + X_1X_2 H_{12} \text{ ……(6)}$$

Tamura- Kurata model [35] - Semi empirical correlation for consideration of viscosity of binary liquid mixture is given by following equation

$$\ln \eta_{12} = X_1 \phi_1 \eta_1 + X_2 \phi_2 \eta_2 + 2(X_1X_2\phi_1\phi_2)^{1/2} T_{12} \text{……(7)}$$

G_{12}, H_{12} and T_{12} are adjustable parameters or interaction parameters calculated from correlation equations and values of these parameters indicate type and extent of interaction. Small standard deviation along with correlation supports the experimental results of viscosity[12].

Table 6: Adjustable parameter for Binary solution of n-AA(1) + isopropanol (2) at 305 to 320 K.

T/K	H_{12}	S	G_{12}	S	T_{12}	S
305 K	0.846	0.0269	-0.0758	0.0298	0.879	0.01404
310 K	0.834	0.0169	-0.0682	0.0244	0.866	0.01048
315 K	0.825	0.0090	-0.0576	0.0237	0.853	0.01800
320 K	0.802	0.0154	-0.0496	0.0247	0.832	0.02765

IV Conclusion

In order to predict the molecular interactions existing in binary solutions of n-amyl acetate with isopropanol, it is necessary to study excess parameters of binaries so that densities and viscosities values measured at different temperatures are employed in calculation for excess molar volume and deviation in viscosity. It is well established that isopropanol molecules are self associated through hydrogen bonding and the breaking of hydrogen bond occurs by the addition of ester to it resulting positive values for excess molar volume. Excess parameters fitted in correlation equation which termed possible interaction in binary solutions. Various

empirical models also employed to correlate viscosity data. Literature reveal that positive value of H_{12} and negative values of G_{12} suggest weak interation between solute-solvent molecules.

References:

[1] Y. W. Sheu and C. H. Tu, "Densities, viscosities, refractive indices, and surface tensions for 12 flavor esters from T = 288.15 K to T = 358.15 K," ***J. Chem. Eng. Data*, vol. 50, no. 5, pp. 1706–1710, 2005**.

[2] F. Karaosmanoglu, K. B. Cıgizoglu, M. Tuter, and S. Ertekin, "Investigation of the Refining Step of Biodiesel Production," ***Energy & Fuels*, vol. 10, no. 4, pp. 890–895, 1996.**

[3] H. Sanei, A. Asoodeh, S. Hamedakbari-Tusi, and J. Chamani, "Multi-spectroscopic investigations of aspirin and colchicine interactions with human hemoglobin: Binary and ternary systems," ***J. Solution Chem.*, vol. 40, no. 11, pp. 1905–1931, 2011.**

[4] L. Guganathan and S. Kumar, "Thermophysical studies of binary liquid mixture of acetate and alkoxyethanols by the Temperature 308.15K," ***Int. J. Mater. Sci.*, vol. 12, no. 2, pp. 89–108, 2017.**

[5] Y. Marcus and G. Hefter, "Standard partial molar volumes of electrolytes and ions in nonaqueous solvents," ***Chem. Rev.*, vol. 104, no. 7, pp. 3405–3452, 2004.**

[6] 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.**

[7] 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.**

[8] A. K. Nain, "Densities and volumetric properties of butyl acrylate + 1-butanol, or +2-butanol, or +2-methyl-1-propanol, or +2-methyl-2-propanol binary mixtures at temperatures from 288.15 to 318.15 K," ***J. Solution Chem.*, vol. 42, no. 7, pp. 1404–1422, 2013.**

[9] N. Indraswati, F. Wicaksana, and H. Hindarso, "Density and Viscosity for a Binary Mixture of Ethyl Valerate and Hexyl Acetate with 1-Pentanol and 1-Hexanol at 293 . 15 K , 303 . 15 K , and 313 . 15 K," ***J. Chem. Eng. Data*, vol. 46, no. 1, pp. 134–137, 2001.**

[10] 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.**

[11] 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.**

[12] 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.**

[13] P. P. Patil, S. R. Patil, a U. Borse, and D. G. Hundiwale, "Density , Excess Molar Volume and Apparent Molar Volume of Binary Liquid Mixtures," ***Rasayan J.Chem.*, vol. 4, no. 3, pp. 599–604, 2011.**

[14] G. W. Brown, "Standard Error," ***Am J. Dis Child*, vol. 136, pp. 937–941, 1982.**

[15] M. V. Rathnam, R. S. Tajuddin, P. J. Sonawane, and M. S. S. Kumara, "Densities,viscosities and speed of sound of n-butyl acetate with toulene at 303.15, 308.15 and 313.15 K: Comparative study on viscosity models," ***Indian J. Pure Appl. Phys.*, vol. 49, pp. 245–250, 2011.**

[16] 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.**

[17] M. N. Roy, B. Sinha, and V. K. Dakua, "Excess molar volumes and viscosity deviations of binary liquid mixtures of 1,3-dioxolane and 1,4-dioxane with butyl acetate, butyric acid, butylamine, and 2-butanone at 298.15 K," ***J. Chem. Eng. Data*, vol. 51, no. 2, pp. 590–594, 2006.**