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Studies on Thermophysical properties of Binary Liquid Mixture of 1-Pentanol and Cyclohexane at Temperature 298.15K

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ABSTRACT

The Thermophysical parameters of densities(ρ), viscosities(η), refractive indices(n_D) and the Excess properties such as Excess molar volume(V^E), Excess viscosity(η^E), deviation of refractive index(Δn_D), Excess molar refraction(Rm^E), Excess Gibbs free energy(ΔG^{*E}) were calculated for the binary mixtures of 1-Pentanol and Cyclohexane at 298.15K. The comparative study of theoretical mixing rule relations for the refractive index of liquids has been carried out. The data obtained from the binary mixture were calculated and the interaction parameters were fitted with Redlich – Kister Polynomial equation. The computed parameters were discussed on the basis of nature of molecular interactions.

Keywords : Densities, Viscosities, Refractive indices, Excess molar refraction, Excess Gibbs free energy

I. INTRODUCTION

The nature and type of interactions in binary organic liquid mixtures have been studied in terms of mixing parameters. These parameters are useful in process engineering, design applications and other related areas[1]. The properties of a system may be divided into two types, namely extensive and intensive. An extensive property of a system is any property whose magnitude depends on the amount of substance present. The properties of liquid mixtures basically depend on its local structure, expressed in terms of packing density, free volume or radial distribution function[2-3]. However, this local structure depends on forces between molecules and their forms and volume of molecules. It changes with compositions. This change in composition changes thermodynamic properties of mixtures[4]. The investigations regarding the molecular association in organic binary mixtures having alkanol group as one of the components is of particular interest, since alkanol group is highly polar and can associate with groups having some degree of polar attractions[5]. My study focuses on ether and alcohol, Alcohols having wide applications in medicine, chemical industry and biology. They are strongly self-associated liquids. The complexes of alcohol symbolize an essential class of hydrogen-bonded solvents. Cyclohexane belongs to alicyclic hydrocarbon (closed chain). The packing of carbon atoms in this even numbered alkane group allows the maximum intermolecular attractions [6].The accessibility of free electrons to do something as a

proton acceptor with alcohols has involved the attention of experimental investigations [7].

1-Pentanol is one of the promising "next generation" alcohol fuels with high energy density and low hygroscopicity. 1-Pentanol is used as a key starting material in the production of dichloro-acetic acid pentyl ester, 2-methyltetrahydrofuran, dinpenyl ether (DNPE), pentyl butyrate and amyl acetate. As a solvent, it is used for coating CDs and DVDs [8]. Cyclohexane is a colourless, mobile liquid with a mild, sweet odour. It is slightly soluble in water and soluble in alcohol, acetone, benzene, etc. It is used as a solvent in some brands of correction fluid. cyclohexane is also used to manufacture esters for plasticizers and synthetic lubricants, as well as produce polyurethanes (synthetic leather) [9].

Moreover, the viscosity(η) is compulsory liquid move from beginning to end cavity surfaces, pipes and for hydraulic computing in energy and mass relocate, in chemical industry. The refractive index is appraised of standard electromagnetic energy. Excess viscosities(η^E), Excess molar volumes(V^E) are frequently applied to investigate molecular interactions in solutions, which assist us to know those actual performances and expand hypothetical models for those explanations on top of the imitation processes. The modern history, we have been the great curiosity in hypothetical and trial investigations of the thermophysical properties of solutions [10]. The Redlich–Kister polynomial equation is applied to recognize the standard deviation in hypothetical and untried values of the liquid solutions. The different theoretical mixing rules are applied in these readings. During investigation, the interaction behavior of 1-Pentanol with Cyclohexane at 298.15K was studied.

II. METHODS AND MATERIAL

a. MATERIALS

Chemicals like 1-Pentanol and Cyclohexane were provided by Loba products (99% Purity), which are utilized without further purification. The purity of chemicals were tested with their literature values such as refractive indices and densities.

b. DENSITY MEASUREMENT

The solutions were taken in airtight closed glass bottles. The weightings were done by using the digital electronic balance. It accuracy is ±0.0001g. Weightings were done at least five times for accuracy of the measurements. The density of pure liquid solutions were utilized by double armed Pycnometer. Pycnometer was calibrated with freshly prepared double distilledwater.

c. VISCOSITY MEASUREMENT

The Viscosities of liquids were employing by Ostwald's Viscometer and calibrated with double distilled water. The rate of flow of liquid in the Viscometer was measured not less than five times for every solution for the better accuracy in measurements. The fluid flow was measured by the stopwatch (Edutek — 19671697), a correctness of accuracy is ±0.01s. The Viscometer was kept in the thermostat for maintaining the fixed temperature 293.15K. The heat was managed to pass around water bath, (supplied by M/s Sakti Scientific Instruments Company,India) and its accuracy is ±0.01K.

d. REFRACTIVE INDEX MEASUREMENT

The refractive index of liquids were taken by the Abbe's refracto meter. It is calibrated by distilled water and ethanol, the uncertainty of refractive index is ± 0.0001.

III. CALCULATIONS

Following are the excess or deviation of the parameters [11-16].

Excess Molar Volume

$V^E = \sum_{i=1}^{n} x_i M_i \ (\rho^{-1} - \rho_i^{-1})$ ……..(1)

Excess Viscosity

$\eta^E = \eta - \sum_{i=1}^{n} x_i \eta_i$ ……..(2)

Deviation of refractive index

$\Delta n_D = n_D - \sum_{i=1}^{n} x_i \ n_{Di}$ ……(3)

Excess Molar refraction

$R_m^E = R_m - \sum_{i=1}^{n} \varphi_i \ R_{mi}$ …….(4)

Excess Gibbs free energy

$\Delta G^{*E} = RT[\ in(V\ \eta) - \sum_{i=1}^{n} x_i \ \ln (V_i \eta_i)]$ …(5)

Where x_i is a symbol of the mole fraction and φ_i is the volume fraction of the pure factor i, correspondingly. ρ, η, n_D, V, and R_m are the density, viscosity, refractive index, molar volume, and molar refraction of the mixtures respectively, and ρ_i, V_i, η_i, n_{Di} and R_i the representational properties of the pure liquids.

$A^E = x_1 (1- \ x_1) \sum_{i=1}^{n} a_i \ \ (2x_{2-} 1)^i$ ……(6)

The Equation(6), excess functions were fitted to Redlich–Kister type polynomial equation and values of coefficient a_i were computed by the method of least squares fit and recognize standard deviation of data based experimental and hypothetical values. The standard deviation data were resumed the equation,

$$\sigma = [\frac{\sum(x_{exp} - x_{cal})^2}{n-p}]^{1/2} \quad \text{……(7)}$$

Here 'n' is the number of experimental data points and 'p' refer to the number ofcoefficients, X_{exp} indicate experimental properties, X_{cal} point out calculated properties.

IV. RESULTS AND DISCUSSION

Here Table 1 reveals the literature and experimental values of 1-Pentanol and Cyclohexane at the temperature 298.15K [17-19].

Table 1. Experimental and literature values of pure Liquids at 298.15K.

S. No	Compounds	ρ/ (kg m^{-3})		η/ (×10^{-3} Nsm^{-2})		n_D	
		Exp.	Lit.	Exp.	Lit.	Exp.	Lit.
1.	1-Pentanol	810.75	810.80	3.4176	3.5128	1.4021	1.4080
2.	Cyclohexane	774.84	773.89	0.8782	0.8799	1.4254	1.4266

Table 2 Shows, the variations of mole fractions of Cyclohexane with increasing the values of viscosities, densities, refractive indices, molar refraction and polarizability. The refractive index is measure in optical region and it must not contribute polarizability of the liquids in orientational effects.

Table 2. Experimental values of density(ρ), viscosity(η), refractive index(n_D), molar refraction(R_m) and polarizability(α) of 1-Pentanol + Cyclohexane binary mixture at 298.15K.

Mole fraction of Cyclohexane X_2	Density ρ (g cm^{-3})	Viscosity η (mPa s)	Refractive Index n_D	Molar refraction R_m (cm^3 mol^{-1})	Polarizability αx10^{-26} (cm mol^{-1})
0.1016	0.9058	0.4215	1.4652	18.5487	0.8124
0.2027	0.9125	0.4302	1.4701	18.9654	0.8321
0.3004	0.9199	0.4398	1.4765	19.3458	0.8457

0.4032	0.9237	0.4419	1.4802	19.7584	0.8569
0.5007	0.9287	0.4489	1.4866	20.2345	0.8655
0.6033	0.9321	0.4520	1.4903	20.7542	0.8798
0.7042	0.9398	0.4601	1.4961	21.4254	0.8936
0.8009	0.9423	0.4685	1.5045	21.9564	0.9088
0.9011	0.9477	0.4731	1.5126	22.5640	0.9196

Here Table 3 Contains excess and deviation of parameters such as V^E, η^E, Δn_D, R^E, and ΔG^{*E} of 1-Pentanol + Cyclohexane binary mixture at 298.15K.

Table 3. Excess molar volume(V^E), excess viscosity(η^E), deviation of refractive index(Δn_D), excess molar refraction(Rm^E) and excess Gibbs free energy(ΔG^{*E}) for 1- Pentanol + Cyclohexane binary mixture at 298.15K.

Mole fraction of Cyclohexane X_2	Excess molar volume V^E ($cm^3\ mol^{-1}$)	Excess viscosity η^E (mPa s)	Deviation of refractive index Δn_D	Excess molar Refraction R^E_m ($cm^3\ mol^{-1}$)	Excess Gibbs free energy ΔG^{*E} ($J\ mol^{-1}$)
0.1016	0.4658	-0.3454	0.0158	0.1854	-356.021
0.2027	0.4758	-0.3521	0.0198	0.1987	-398.002
0.3004	0.4821	-0.3603	0.0236	0.2145	-448.332
0.4032	0.4945	-0.3758	0.0298	0.2450	-564.654
0.5007	0.5122	-0.3885	0.321	0.2584	-624.854
0.6033	0.5265	-0.4021	0.0406	0.2782	-714.360
0.7042	0.4818	-0.3650	0.0240	0.2254	-398.334
0.8009	0.4754	-0.3587	0.0264	0.2365	-412.330
0.9011	0.4656	-0.2502	0.0275	0.2400	-135.445

The Excess molar volume(V^E) values are positive and excess viscosity(η^E) values are negative in system. The excess molar volume(V^E) increases as the chain length of 1-Pentanol increases. The excess molar volume(V^E) has high positive readings which are located between 0.4 and 0.6 Mole fractions of Cyclohexane. The highest positive readings of the whole range of the systems are present in the liquid mixture. It may be attributed to supremacy of molecular dissociation[20].

The shows that excess viscosity(η^E) increasing as the chain length of 1-Pentanol increases. These excess viscosity readings are negative; whereas the highest negative readings are located between 0.4 to 0.6 mole fractions. The excess viscosity(η^E) readings are found to be opposite to the sign of excess molar volume V^E for the binary mixtures, which is in agreement with the views proposed [21-22]. A correlation between the sign (η^E) and (V^E) has been observed for a number of binary system; (i.e.) (η^E) negative when (V^E) is positive and vice– versa [23-24].

The deviations of refractive index shows(Δn_D) positive for the whole system. These positive readings are due to the strong specific forces between the participated molecules, such as hydrogen bonding between the constituent molecules.

In the (Table 3), the excess molar refraction(R_m^E) shows the highest positive readings. Which are located between 0.4 and 0.6 mole fractions of Cyclohexane, the order of magnitude and change of sign indicates the size variation between one and the same molecules. The Excess Gibbs free energy(ΔG^{*E}) deals with the molecular interactions of fluid mixtures. The negative reading shows the dispersion forces between the molecules. From (Table 4), the readings of adjustable parameters and standard deviations of Redlich–Kister polynomial equations[10]. The readings of standard deviations are giving the acceptable outcome for the experimental readings. The experimental refractive index readings are examined by seven theoretical mixing rules [25-27].

Table 4. Values of adjustable parameters(B_k) and the corresponding standard deviations(σ), for excess molar volumes(V^E), excess viscosity(η^E), deviation of refractive index(Δn_D), excess molar refraction(Rm^E) and excess Gibbs free energy(ΔG^{*E})for 1- Pentanol + Cyclohexane binary mixture at 298.15K.

Parameters	B_k							σ
	B_0	B_1	B_2	B_3	B_4	B_5	B_6	
V^E (cm^3 mol^{-1})	2.0365	0.1145	-1.9654	-0.3045	4.6872	0.2154	-5.2548	2.8972
η^E (mPa s)	-1.1472	-0.2536	1.4875	0.2654	-2.5587	0.0458	3.2548	0.3654
R_m^E (cm^3 mol^{-1})	1.9889	-0.3654	-2.2145	0.3548	4.9968	0.0754	-5.2542	1.5485
Δn_D	0.0885	-0.00987	-0.0887	0.0025	0.1245	0.0087	-0.0987	0.0123
ΔG^{*E} (J mol^{-1})	-2012.6655	-2145.3212	2654.2588	658.2143	-5421.2216	1854.3897	4218.3477	601.7549

Table 5. Values of standard deviation for refractive index by different theoretical mixing rules for 1-Pentanol + Cyclohexane binary mixture at 298.15K.

Standard deviation σ							
System	L–L	Wiener	G–D	A–B	Heller	Newton	Oster
1-Pentanol + Cyclohexane	0.0094	0.0081	0.0174	0.0147	0.0129	0.0318	0.0354
L–L: Lorentz–Lorentz; G–D: Gladstone–Dale; A–B: rago–Biot							

The standard deviation is computed and reported in (Table 5). Theoretical mixing rules like Lorentz–Lorenz(L–L), Arago–Biot(A–B), Newton, Gladstone–Dale(G–D), Heller(H), Weiner(W) and Oster deals with predicting the refractive index of a fluid. It has been accomplished and validity for the liquid binary mixture. The presentation of the theoretical mixing rules of Weiner(W) has small deviation while Oster and Newton's has comparatively higher deviation values. The deviations indicate that values of the experimental and theoretical are almost nearby. The deviations are less than 2% for the calculated binary systems [25].

V. CONCLUSION

Thermophysical parameters such as viscosity (η), density (ρ) and the refractive index (n_D) were calculated from 1-Pentanol + Cyclohexane binary mixture at 298.15K. The excess properties such as Excess molar volume (V^E), Excess viscosity(η^E), deviations of refractive index (Δn_D), Excess molar refraction(R_m^E) and Excess Gibbs free energy(ΔG^{*E}) readings were calculated and fitted with Redlich–Kister polynomial equations. Hence from the presentations of theoretical mixing rules of Oster and Newton's readings were comparatively maximum deviations than that of other theoretical mixing rules.

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