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Study of Molecular Interactions of 2-(Dimethylamino) Ethanol with some higher Alcohols at 298.15K

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Abstract: **Viscosity(η), density(ρ), and ultrasonic velocity of 2-(Dimethylamino) ethanol with 1-butanol,1-pentanol, and 1-hexanol binary system of different compositions at 298.15 K were studied. The viscosity, density, and ultrasonic velocity data are used for the determination of excess molar volume (V^E), the viscosity deviation (Δη), and isentropic compressibility(ΔKs). These values were fitted with Redlich-Kister type polynomial equation. The value of viscosity was observed to decreases with an increase in concentration in the case of 1-Butanol and 1-Pentanol but a reverse trend is observed in the case of 1-Hexanol. A significant decrease in ultrasonic velocity was observed with increase concentration in the case of 1-Butanol and 1-Pentanol. The positive value of isentropic compressibility (ΔKs) for 2-(Dimethylamino) ethanol with a 1-butanol binary system is due to stronger polar interactions.**

Index Terms: **Viscosity, Density, Ultrasonic velocities.**

I. INTRODUCTION

Molecular interactions play an important role in liquid mixtures. They affect the arrangement, orientation, and conformation of molecules in solutions. Ultrasonic energy is very useful in agriculture, medicine, engineering, and industry (Chauhan S. K, et al.,1993; Blokhra, R.L., et al.,1991). The Viscosity (η), Density (ρ), and Ultrasonic velocities (U) measurements find wide applications in characterizing the physicochemical behavior of liquid mixtures (Kinocid 1929; Mehra. K. S ,2000; Fort, R.J.et al.,1965).

2-(Dimethylamino)ethanol is a bifunctional compound containing both tertiary amine and primary alcohol functional groups. Amino-alcohols are bi-functional organic compounds having two kinds of polar groups, hydroxyl and amino groups, leading to complicated intermolecular interactions with the molecules having polar groups. They are used as chemical intermediates for the pharmaceutical industry (Lagemann R.T. et al.,1945; Puneet K.et al.,2013; Hawrylak, B., et al.,2000; Bernal-Garcfa, et al.,2005). In multifunctional molecules, the exact hydrogen bonding with suitable molecule will result in micro and complicated competition between various possibilities, so the binary system of 2-(Dimethylamino) ethanol with 1-butanol,1-pentanol, and 1-hexanol are of considerable interest for finding the intra and intermolecular behavior of the present solvent system.

In this study, the measurement of viscosity, density, and ultrasonic velocity of a binary mixture of 2-(Dimethylamino) ethanol with 1-butanol,1-pentanol, and 1-hexanol at different compositions and at 298.15 K was carried out.

II. MATERIAL AND METHODS

2-(Dimethylamino) ethanol, 1-butanol,1-pentanol, and 1-hexanol used are 99% pure from E-Merck, Germany, and Sd Fine chemicals, India, without purification. The measured viscosities, densities, and ultrasonic velocities were compared with literature values, and the comparison is recorded in Table-1. The purities of the above chemicals were checked by density determination at 298.15K the uncertainty is less than ± $1x10^{-4}$ gcm^{-3}. The binary liquid mixtures of different known compositions were prepared in stopper measuring flasks. The density, viscosity, and ultrasonic velocity were measured as a function of the composition of the binary liquid mixture of 2-(Dimethylamino) ethanol, 1-butanol,1-pentanol and 1-hexanol respectively at 298.15 K. The density was determined using a Bi-capillary pyknometer. The weight of the sample was measured using an electronic digital balance with an accuracy of ± 0.1 mg (Model: Shimadzu AX-200). An Ubbelohde viscometer (20ml) was used for the viscosity measurement and efflux time was determined using a digital clock to within ±0.01s. An ultrasonic interferometer having the frequency of 2 MHz (Mittal Enterprises, New Delhi, Model: F-81) with an overall accuracy of ± 0.1% has been used for velocity measurement. An electronically digital operated constant temperature bath (RAAGA Industries) has been used to circulate water through the

double-walled measuring cell made up of steel containing the experimental solution at the desired temperature with an accuracy of ± 0.01 Excess volumes are determined by

$$V^E = (M_1X_1+M_2X_2) / \rho_{12} - (M_1X_1) / \rho_1 - (M_2X_2) / \rho_2 \quad (1)$$

The viscosity of Binary Mixtures is determined by:

$$\ln \eta_m = X_1 \ln \eta_1 + X_2 \ln \eta_2 \quad (2)$$

Deviation in Viscosity of Binary Mixtures is determined by :

$$\Delta\eta_m = \eta_{12} - X_1 \eta_1 - X_2 \eta_2 \quad (3)$$

Deviation in isentropic compressibility have been evaluated by using the equation ,

$$\Delta K_S = K_S - (\Phi_1 K_{S1} + \Phi_2 K_{S2}) \quad (4)$$

Where k_{S1}, k_{S2} and K_S are isentropic compressibility of liquid mixtures and Φ is the volume fraction of pure components.

The excess properties yE are fitted by the method of nonlinear least squares to a Redlich kister type polynomial

$$y^E = X_1 X_2 \Sigma Ai (X_1 - X_2) i \quad (5)$$

In each case, the optimum number of coefficients Ai was determined from an examination of the variation of standard deviation as calculated by:

$$\sigma y^E = [\Sigma (y^E obs - Y^E cal) / (n-m)]1/2 \quad (6)$$

Where n represents the number of experimental points and m represents the number of coefficients in fitting the data.

III. RESULT AND DISCUSSION

To study the various interaction parameter such as viscosity(η), density(ρ), and ultrasonic velocity for 2 -(Dimethylamino) ethanol with 1-butanol,1-pentanol, and 1-hexanol binary mixed system at different compositions and hexanol binary mixed system at different compositions and at 298.15 K were studied and data are compiled in Table 1-4.

The viscosity, density, and ultrasonic velocity data are used to calculate excess molar volume (V^E), the viscosity deviation (Δη), and isentropic compressibility(ΔKs) for the above-mentioned binary system and are compiled in Table 5-7.

The observed experimental data of viscosity(η), density(ρ), and ultrasonic velocity are comparable with the literature values at different temperatures is mentioned in Table 1. The experimental values are in good agreement with the literature values.

The observed values such as density (ρ), viscosity (η), ultrasonic velocity (U), viscosity deviation (Δη), excess molar volume (V^E), deviation in isentropic compressibility (ΔK_S), are given in Table-2, Table-3and Table-4 respectively. Excess free length (L_f^E), Internal pressure (π^E), available volume (V_a^E) and Gibbs free energy (G^{*E}) are given in Table-5, Table-6, and Table-7 respectively.

As the concentration of 2-(Dimethylamino) ethanol increases and the concentration of 1-Butanol,1-Pentanol decreases the viscosity, density, ultrasonic velocity, excess volume increases.

Table-I: Comparison of experimental values of viscosity, density, and ultrasonic velocity of 2-(Dimethyl-amino) ethanol 1-Butanol,1-Pentanol, and 1-Hexanol with literature values.

Chemical	T (K)	ρ × 10^{-3}(Kg·m^{-3})		η(mPa·s)		U (m·s^{-1})	
		Exp.Value	Lit. Value	Exp.Value	Lit. Value	Exp.Value	Lit. Value
2-(Dimethyl- amino)ethanol	298.15	0.88310	0.88257[8]	3.34618	3.381[11]	1354.20	1344.4[7]
			0.88334[9]				
			0.88300[11]				
	303.15	0.87885	0.87835[8]	2.9670	2.959[11]	1351.90	1326.7[7]
			0.879315[10]		2.96[12]		
			0.87880[11]				
	308.15	0.87518	0.87546[9]	2.54123	2.595[11]	1349.50	1309.1[13]
			0.875017[10]		2.59[12]		
			0.87450[11]				
1-Butanol	298.15	0.79941	0.80788	2.565615	2.5180	1266.20	1251.78
							1242.6
	303.15	0.79670	0.80221	2.27852	2.296	1192.80	1225.64
	308.15	0.79268	0.79834			1191.20	1220.4
1-Pentanol	298.15	0.80435	0.81094	3.51431	3.510	1268.60	1275.32
			0.81090		3.5128		
	303.15	0.80094	0.8020	2.46151	3.034	1264.60	1260.0
					2.798		
	308.15	0.79756	0.80383	2.32620	2.648	1262.20	1250.8
					2.73		
1-Hexanol	298.15	0.80807	0.8153	4.59266	4.477	1271.30	-
			0.81523		4.339		
	303.15	0.80510	0.81170	3.9189	3.7009	1270.20	1284.82
			0.81160		3.8610		1287.9
					3.7690		
	308.15	0.8007	0.8082	3.3645	3.413	1269.40	-
					3.398		

In the case of 1-Hexanol, the increase in concentration of 2-(Dimethylamino) ethanol and decrease in the concentration of 1-Hexanol, density and ultrasonic velocity increases but the viscosity and viscosity deviation decrease (Figure 1). This decrease in value may be due to the long chain of 1-hexanol and hydrophobic interaction. They reported that the values of ΔK_S are positive over the range of composition for 2-(Dimethylamino) ethanol + 1-Butanol and 2-(Dimethylamino) ethanol + 1-Pentanol binary system leading to an increase in free length, which may be due to the existence of weak dipolar interactions between the polar hydroxy group of butanol and pentanol molecules with polar 2-(Dimethylamino)ethanol. The negative values of ΔK_S is observed over the range for 2-(Dimethylamino) ethanol + 1-Hexanol binary system shows negative values of free length, which may be due to hydrophobic interaction. A similar trend was also reported by Kannappan et al (Kannappan A N & Rajendran,1990)

Table-II: Values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations and (Δη), deviation on isentropic compressibility (Δk_S) for Binary System of 1-Butanol and 2-(Dimethyl-amino) ethanol at 298.15 K.

Temp. (K)	X_1	ρ(gm/cm^3)	η x10^3 (Nsm^{-2})	U (M S^{-1})	V^E x10^6(m^3 mole^{-1})	Δη x 10^3 (Kg m^{-1} s^{-1})	ΔK_S x 10^{11}(m^2 N^{-1})
298.15	0.0000	0.79941	2.56562	1266.2	0.0000	0.000	0.00
	0.0847	0.80245	2.66177	1267.4	0.5382	2.979	10.41
	0.1722	0.81044	2.835236	1268.6	0.5132	13.495	16.46
	0.2628	0.81824	3.083858	1270.6	0.5293	31.285	22.21
	0.3565	0.83531	3.569804	1272.1	0.5063	72.566	20.71
	0.4540	0.83631	3.70979	1274.5	0.3304	78.954	24.15
	0.5547	0.83968	4.08914	1277.3	0.6448	109.029	43.33
	0.6598	0.85641	4.36211	1344.7	0.3445	128.122	48.12
	0.7686	0.86018	5.197343	1349.1	0.5508	203.152	34.10
	0.8809	0.86469	5.891789	1351.1	1.0588	263.831	32.02
	1.0000	0.88310	3.346187	1354.2	0.0000	0.000	0.00

Table-III: Values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations and(Δη), deviation on isentropic compressibility (Δk_S) for Binary System of 1-Pentanol and 2-(Dimethylamino)ethanol at 298.15,303.15 and 308.15K

Temp. (K)	X_1	P (gm/cm^3)	η x10^3 (Nsm^{-2})	U (M S^{-1})	V^E x10^6 (m^{3}mole^{-1})	Δη x 10^3 (Kg m^{-1} s^{-1})	Δk_S x 10^{11}(m^2 N^{-1})
298.15	0.0000	0.80435	3.514369	1268.6	0.0000	0.000	0.00
	0.0992	0.813819	3.557358	1269.8	-0.2964	1.973	-1.80
	0.1983	0.81784	3.606061	1270.3	0.1479	4.554	2.71
	0.2979	0.820109	3.684134	1271.2	0.8309	10.061	8.56
	0.3974	0.833248	3.742837	1272.5	0.8692	13.634	4.31
	0.4973	0.834586	3.922069	1276.9	0.9217	29.250	7.39
	0.5975	0.841755	4.426034	1283.3	1.0018	77.332	3.41
	0.6977	0.848628	4.919149	1308.7	1.1316	124.329	-20.25
	0.7981	0.879283	5.795549	1347.9	-1.5369	209.651	-72.43
	0.8990	0.888825	6.40794	1351.9	-1.6376	268.559	-72.71
	1.0000	0.80435	3.746187	1354.2	0.0000	0.087	0.00

Table-IV: Values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations and (Δη), deviation on isentropic compressibility (Δk_S) for Binary System of 1-Hexanol and 2-(Dimethylamino) ethanol at 298.15 K

Temp. (K)	X_1	ρ(gm/cm^3)	η x10^3 (Nsm^{-2})	U (M S^{-1})	V^E x10^6(m^3 mole^{-1})	Δη x 10^3 (Kg m^{-1} s^{-1})	Δk_S x 10^{11}(m^2 N^{-1})
298.15	0.0000	0.80807	4.592668	1271.3	0.0000	0.000	0.00
	0.1130	810990	4.665151	1344.3	0.6395	21.288	7.67
	0.2228	0.836987	4.510738	1346.3	1.1565	19.533	-90.26
	0.3294	0.827732	4.423123	1345.1	0.2097	24.059	-73.32
	0.4332	0.831547	4.140797	1345.5	0.6873	8.765	-68.24
	0.5342	0.836951	4.003162	1345.5	0.9405	7.591	-63.84
	0.6323	0.856105	3.985871	1346.3	-0.5968	18.089	-70.56
	0.7278	0.856114	3.832161	1346.3	0.3836	14.622	-61.58
	0.8204	0.879283	3.713349	1346.3	-1.4807	14.284	-69.44
	0.9116	0.862883	3.419866	1373.9	1.4451	-3.697	26.61
	1.0000	0.80435	3.346187	1354.2	0.0000	0.000	0.00

Table-V: Values of Excess Free Length (L_f^E), Internal Pressure (π^E), Available Volume (Va^E), and Gibbs free energy(G^{*E}) of Binary System of 1- Butanol and 2-(Dimethylamino) ethanol at 298.15K.

Temp.K	X_1	L_f^E x 10^{-10} m	V_a^E x 10^{-6}m^{3}mol^{-1}	π^E x 10^6 Nm^{-1}	G^{*E} Jmol^{-1}
298.15K	0.0000	0.000	0.000	0.0	0.0
	0.0847	0.004	0.512	372.7	49.3
	0.1722	0.006	0.921	2196.1	148.0
	0.2628	0.008	1.307	4885.3	297.5
	0.3565	0.007	1.523	11145.3	571.9
	0.4540	0.012	2.087	11332.2	624.8
	0.5547	0.016	2.589	14430.4	814.5
	0.6598	-0.010	-1.157	14627.8	881.5
	0.7686	-0.006	-0.778	21593.8	1258.1
	0.8809	-0.001	-0.249	26477.8	1506.7
	0.0000	0.000	0.000	0.0	0.0

Table-IV: Values of Excess Free Length (L_f^E), Internal Pressure (π^E), Available Volume (Va^E), and Gibbs free energy(G^{*E}) of Binary System of 1- Pentanol and 2-(Dimethylamino) ethanol at 298.15K.

Temp.K	X_1	L_f^E x 10^{-10} m	V_a^E x 10^{-6}m^{3}mol^{-1}	π^E x 10^6 Nm^{-1}	G^{*E} Jmol^{-1}
298.15K	0.0000	0.000	0.0000	1061.2	7.2
	0.0992	0.002	0.242	1864.7	36.0
	0.1983	0.004	0.686	2864.4	89.6
	0.2979	0.003	1.153	4356.5	96.8
	0.3974	0.004	1.306	6276.1	216.1
	0.4973	0.002	1.570	11879.4	502.0
	0.5975	-0.007	1.558	16376.0	751.0
	0.6977	-0.027	0.319	25415.4	1076.9
	0.7981	-0.028	-2.234	31377.5	1306.6
	0.8990	0.000	-2.065	1061.2	7.2
	1.0000	0.000	0.000	0.0	0.0

Table-VII: Values of Excess Free Length (L_f^E), Internal Pressure (π^E), Available Volume (Va^E) and Gibbs Free Energy(G^{*E}) of Binary System of 1- Hexanol and 2-(Dimethylamino) ethanol at 298.15K.

Temp.K	X_1	L_f^E x 10^{-10} m	V_a^E x 10^{-6}m^{3}mol^{-1}	π^E x 10^6 Nm^{-1}	G^{*E} Jmol^{-1}
298.15K	0.0000	0.000	0.000	0.000	0.000
	0.1130	-0.033	-4.966	1761.4	-41.2
	0.2228	-0.026	-5.176	2057.8	94.7
	0.3294	-0.024	-4.189	2303.8	181.9
	0.4332	-0.022	-3.635	1493.5	111.9
	0.5342	-0.025	-3.100	2016.9	113.7
	0.6323	-0.022	-2.919	4499.0	145.2
	0.7278	-0.026	-2.295	4416.8	142.9
	0.8204	0.011	-2.136	6042.0	90.5
	0.9116	-0.054	3.510	5405.1	23.2
	1.0000	0.000	0.000	0.0	0.0

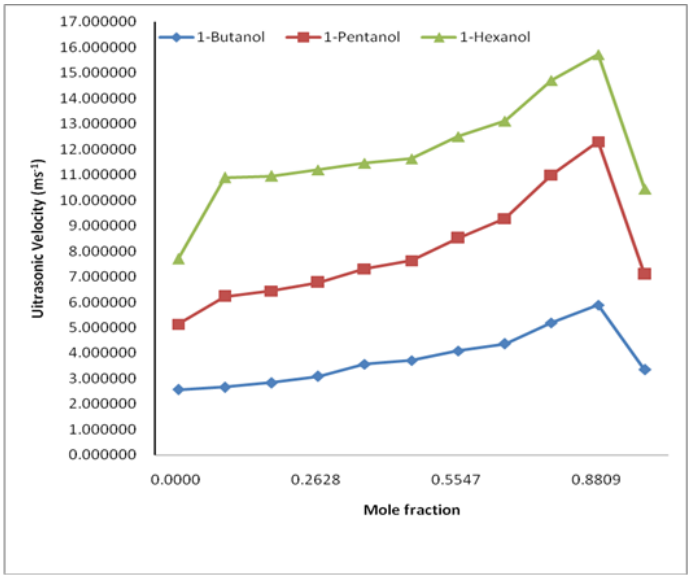

Fig.1: Graph of Viscosity (η) Vs Mole fraction(X_1) of binary system of 2-(Dimethylamino) ethanol and 1-Butanol, 1-Pentanol and 1-Hexanol at 298.15K.

CONCLUSION

The value of viscosity was observed to decreases with an increase in concentration in the case of 1-Butanol and 1-Pentanol but a reverse trend is observed in the case of 1-Hexanol is due to an increase in hydrophobic interaction will decrease the polar–polar ,interaction. A significant decrease in ultrasonic velocity was observed with increase concentration in presence of 1-Butanol and 1-Pentanol. The positive value of isentropic compressibility (ΔK_S) for 2-(Dimethylamino) ethanol with a 1-butanol binary system is due to stronger dipole-dipole interactions. The overall observed changes in thermoacoustic parameters indicate that the increase in chain length of n-alcohols in the presence 2-(Dimethylamino)ethanol binary system shows a decreased dipole-dipole interaction is due to the increase in hydrophobicity of n-alcohols.

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