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Intermolecular Interactions of Brompheniramine with 1-Pentanol at Various Temperatures.

Sampandam Elangovan*, Kumera Assefa and Yilak Alemu Abbo
Department of Physics, Wollega University, Nekemte, Ethiopia.

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ABSTRACT
Ultrasonic velocity (U), viscosity (η) and density (ρ), were measured for liquid mixtures of Brompheniramine and1-pentanol at 303,308 and 313K. Adiabatic compressibility (β), viscous relaxation time (τ), free volume (V_f), free length (L_f), and Gibbs free energy (ΔG) were determined. Excess values of that parameters (β^E, L_f^E , V_f^E ,τ^E and ΔG^E) also calculated and elucidated in terms of intermolecular interaction like hydrogen bond between selected liquid system. It was observed that homo and hetero association of molecules decreased with the temperatures.

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Introduction

Ultrasonic velocity changed with liquid medium and intermolecular interaction between the liquid mixtures. Physical parameters like density, viscosity also changed with liquid system. It is one of the reliable techniques to analyze the molecular interaction of the selected liquid mixtures. It takes vital role in the chemical and pharmaceutical industries [1-5].Brompheniramine is used in common cold, allergic rhinitis. 1-pentanol is highly polar and self-associated in nature. Hence the useful interaction may obtain in the liquid system present with alcohols as one of the medium [6-8]. Here molecular interaction between brompheniramine and 1-pentanol at 303,308 and 313K was determined by ultrasonic data.

MATERIALS AND METHODS

Various concentrations of liquid mixtures were prepared in standard flasks with air tight caps. Masses of the system were determined by digital electronic balance (ACM-78094L,ACMAS Ltd, India) with accuracy of ±1mg. Density and viscosity were measured by specific gravity bottle and Ostwald's viscometer with accuracy ±0.01kgm^{-3} and ±0.001Nsm^{-2} .Ultrasonic velocities in the liquid mixtures were determined by a single crystal ultrasonic interferometer (Mittal Enterprizes,New Delhi Model:f81) operated at 2MHZ. Accuracy was ±1ms^{-1}. Liquid system was maintained in a constant temperature bath [INSREF model IRI-016C,India] with accuracy ±0.01K.Brompheniramine was obtained from Varda Biotech Pvt.ltd, Mumbai, India.AR grade 1-pentanol with mass fraction purities greater than 99% was used without further purification

THEORY

Ultrasonic velocities have been measured by using the following relation

Ultrasonic velocity $U = f\lambda$ (1)

Here f is ultrasonic frequency and λ is ultrasonic wavelength.

Adiabatic compressibility

$$\beta = \frac{1}{U^2\rho} \quad (2)$$

Where U is ultrasonic velocity and ρ is density of the liquid mixture.

Free length $L_f = K_T\sqrt{\beta}$ (3)

Where K_T is the temperature dependent constant having the following values in M.K.S system

TABLE 1.The K_T values at different temperatures.

Temperature (T) K	K_T M.K.S
303	1.9953 ×10^{-6}
308	2.01121×10^{-6}
313	2.03018×10^{-6}

Free Volume

$$V_f = \left[\frac{M_{eff}U}{\eta K}\right]^{3/2} \quad (4)$$

Where M_{eff} is the effective molecular weight ($M_{eff}=m_1x_1+m_2x_2+m_3x_3$) m and x are molecular weight and mole fraction of the individual liquid components. η is the viscosity of the solution is a temperature dependent constant which is equal to 4.28×10^9 for all liquid system.

Viscous relaxation time

$$\tau = \frac{4}{3}\beta\eta \quad (5)$$

Here β is the compressibility of the liquid mixtures and η is co efficient of viscosity of the liquid mixtures.

Gibbs free energy

$$\Delta G = kT\ln\left(\frac{kT\tau}{h}\right) \quad (6)$$

Excess values of the acoustic parameters have been calculated using the following equation,

Tele:
E-mail address: elangovan.physics@rediffmail.com

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TABLE 2. Physical and acoustical parameters of brompheniramine and 1-pentanol at 303K,308K and 313K.

X_1	ρ (Kgm^{-3})	η × 10^{-3} (Nsm^{-2})	U (ms^{-1})	β ×10^{-10} (m^2N^{-1})	L_f ×10^{-10} (m)	V_f × 10^{-8} (m^3mol^{-1})	τ × 10^{-12} (s)	ΔG × 10^{-20} ($KJmol^{-1}$)
T=303K								
0.0000	803.2	1.9747	1227.8	8.2588	0.5734	0.222	2.1745	1.0708
0.0311	821.2	2.0227	1255.2	7.7290	0.5547	0.2416	2.0844	1.0524
0.0757	841.7	2.0776	1286.6	7.17721	0.5345	0.2655	1.9881	1.0318
0.1274	865.5	2.1412	1323	6.6010	0.5126	0.295	1.8845	1.0084
0.1879	893.4	2.2157	1365.6	6.0021	0.4888	0.3317	1.7732	0.9820
0.2596	926.4	2.3039	1416	5.3836	0.4629	0.3782	1.6537	0.9517
0.3460	966.2	2.4102	1476.8	4.7455	0.4346	0.4383	1.5250	0.9165
0.4521	1015.1	2.5408	1551.5	4.0924	0.4036	0.5177	1.3864	0.8753
0.5857	1076.6	2.7052	1645.5	3.4304	0.3695	0.6258	1.2373	0.8261
0.7588	1156.3	2.9182	1767.3	2.7689	0.3320	0.7782	1.0773	0.7664
1.0000	1263.8	3.2053	1931.5	2.1209	0.2905	1.0038	9.0644	0.6921
T=308K								
0.0000	800.9	1.6882	1209.7	8.5323	0.5874	0.2428	1.9205	1.0493
0.0311	818.8	1.7299	1236.8	7.9840	0.5682	0.2666	1.8415	1.0305
0.0757	839.3	1.7776	1267.7	7.4139	0.5476	0.2956	1.7572	1.0096
0.1274	863.1	1.8328	1303.6	6.8178	0.5251	0.3313	1.6661	0.9859
0.1879	890.9	1.8975	1345.6	6.1992	0.5007	0.3758	1.5684	0.9589
0.2596	923.9	1.9741	1395.4	5.5587	0.4741	0.4322	1.4631	0.9281
0.3460	963.7	2.0665	1455.4	4.8988	0.4451	0.505	1.3497	0.8923
0.4521	1012.5	2.1799	1529.1	4.2240	0.4133	0.6011	1.2277	0.8503
0.5857	1073.9	2.3227	1621.8	3.5403	0.3784	0.732	1.0964	0.8003
0.7588	1153.5	2.5077	1742	2.8568	0.3399	0.9166	9.5521	0.7396
1.0000	1260.8	2.7571	1904	2.1878	0.2974	1.1900	8.0428	0.6641
T=313K								
0.0000	797.3	1.4541	1197.1	8.7520	0.6006	0.2671	1.6968	1.0271
0.0311	815.3	1.4908	1224	8.1869	0.5808	0.2958	1.6273	1.0079
0.0757	835.8	1.5328	1254.8	7.5988	0.5596	0.3306	1.553	0.9865
0.1274	859.6	1.5814	1290.5	6.9853	0.5365	0.3736	1.4728	0.9623
0.1879	887.5	1.6383	1332.3	6.3478	0.5115	0.4272	1.3866	0.9348
0.2596	920.5	1.7058	1381.8	5.6896	0.4842	0.495	1.2940	0.9033
0.346	960.3	1.7871	1441.5	5.0114	0.4544	0.5826	1.1941	0.8668
0.4521	1009.1	1.887	1514.7	4.3192	0.4219	0.6982	1.0867	0.8241
0.5857	1070.7	2.0127	1607	3.616	0.3860	0.8556	9.7055	0.7730
0.7588	1150.4	2.1756	1726.5	2.9162	0.3466	1.0776	8.4593	0.7111
1.0000	1257.8	2.3951	1887.6	2.2313	0.3032	1.4062	7.1257	0.6341

$A^E=A_{exp}-A_{id}$ (7)

$A_{id}=x_1 A_1+x_2A_2$

Here x_1 and x_2 are mole fractions of brompheniramine and 1-butanol respectively.A_1 and A_2 are acoustical parameters.

RESULT AND DISCUSSION

Density (ρ), viscosity (η), ultrasonic velocity (U) and calculated values of adiabatic compressibility (β), free length (L_f), free volume (V_f), viscous relaxation time (τ) , Gibbs free energy (ΔG) for a binary mixture of brompheniramine and 1-pentanol at 303K,308K and 313K were listed in table 2.

It is noticed that density (ρ) increased with increasing concentration of brompheniramine. When the temperature increased, density was decreased in the liquid mixture. It is also reflected in viscosity values. It signifies that the system is more compact [9].

Mole fraction of brompheniramine increases the net dispersive interactions and hence the ultrasonic velocity continuously increased as shown in the fig1.It shows that ultrasonic velocity decreases with increase in temperature. It may due to thermal agitation in the liquid system [10]. Adiabatic compressibility (β) is decreased with increasing concentrations of brompheniramine in the 1-pentanol.It signifies that specific interaction takes place in the liquid system.[10]

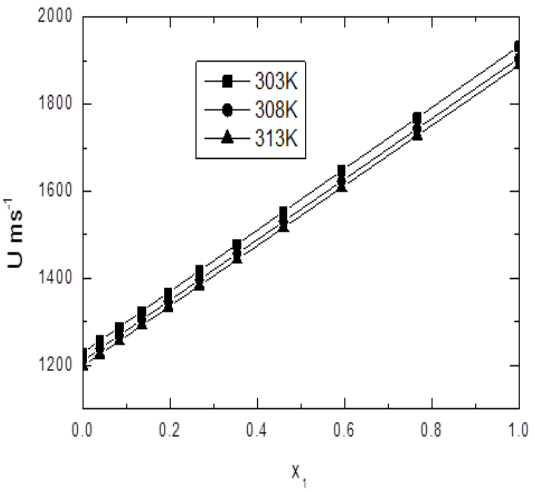

FIGURE 1. Variation of ultrasonic velocity (U) with the mole fraction of brompheniramine.

TABLE 3.Excess parameters of brompheniramine with 1-pentanol at various temperatures.

x_1	β^E $\times 10^{-10}$ (m^2N^{-1})	L_f^E $\times 10^{-11}$ (m)	V_f^E $\times 10^{-9}$ (m^3mol^{-1})	τ^E $\times 10^{-12}$ (s)	ΔG^E $\times 10^{-21}$ ($KJmol^{-1}$)
T=303K					
0.0000	0.0123	0.0123	0.0123	0.0123	0.0123
0.0390	-0.2767	-0.0637	-0.0966	-0.0336	-0.0240
0.0836	-0.5533	-0.1389	-0.2063	-0.0784	-0.0611
0.1353	-0.8108	-0.2120	-0.3155	-0.1212	-0.0993
0.1958	-1.0372	-0.2783	-0.4215	-0.1599	-0.1342
0.2675	-1.2148	-0.3341	-0.5170	-0.1916	-0.1657
0.3539	-1.3221	-0.3723	-0.5915	-0.2127	-0.1905
0.4600	-1.3240	-0.3830	-0.6270	-0.2166	-0.2007
0.5936	-1.1669	-0.3462	-0.5905	-0.1934	-0.1867
0.7667	-0.7681	-0.2318	-0.4198	-0.1265	-0.1282
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=308K					
0.0000	0.0123	0.0123	0.0123	0.0123	0.0123
0.0390	-0.2869	-0.0669	-0.1191	-0.0289	-0.0255
0.0836	-0.5725	-0.1438	-0.2516	-0.0689	-0.0627
0.1353	-0.8392	-0.2183	-0.3843	-0.1073	-0.1005
0.1958	-1.0729	-0.2863	-0.5123	-0.1419	-0.1375
0.2675	-1.2575	-0.3438	-0.6275	-0.1706	-0.1693
0.3539	-1.3688	-0.3839	-0.7178	-0.1896	-0.1945
0.4600	-1.3705	-0.3939	-0.7618	-0.1931	-0.2058
0.5936	-1.2076	-0.3554	-0.7183	-0.1721	-0.1912
0.7667	-0.7950	-0.2386	-0.5119	-0.1122	-0.1314
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=313K					
0.0000	0.0123	0.0123	0.0123	0.0123	0.0123
0.0390	-0.2970	-0.0690	-0.1449	-0.0249	-0.0264
0.0836	-0.5927	-0.1487	-0.3050	-0.0612	-0.0652
0.1353	-0.8677	-0.2254	-0.4639	-0.0958	-0.1040
0.1958	-1.1094	-0.2960	-0.6171	-0.1272	-0.1412
0.2675	-1.2992	-0.3553	-0.7558	-0.1529	-0.1744
0.3539	-1.4135	-0.3960	-0.8640	-0.1700	-0.1999
0.4600	-1.4139	-0.4053	-0.9166	-0.1729	-0.2099
0.5936	-1.2463	-0.3671	-0.8644	-0.1542	-0.1959
0.7667	-0.8202	-0.2467	-0.6162	-0.1001	-0.1346
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

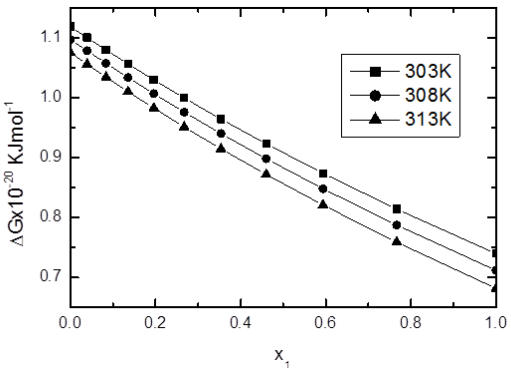

FIGURE 2. Variation Gibbs free energy with brompheniramin.

Moreover intermolecular free length (L_f) decreased with concentration of alcohol and temperature elucidates that closer packing of molecules in the selected liquid mixture. Free volume (V_f) also in the same trend, it suggests that hydrogen bonding takes place in the interactions. Viscous relaxation time (τ) decreased with the temperature and mole fraction of the brompheniramine .It may be due to dissociation in the higher concentration of alcohol.

Reduction of free energy (ΔG) with the concentration of brompheniramine and temperature is as shown in the figure2.The curves signify that disassociation of the molecules in the liquid mixture.

Determination of excess parameters was useful to identify the nature of interaction of the liquid mixtures. It is noted that positive excess values araised due to the dispersion interaction and negative of the excess values signifies that the dipole-dipole and hydrogen bonding interactions formed in the liquid system.

Excess adiabatic compressibility (β^E), excess free length (L_f^E), excess free volume (V_f^E),excess viscous relaxation time (τ^E) and excess Gibbs free energy (ΔG^E) are listed in table3.

All the negative values of excess parameters confirm formation of hydrogen bond between the N-H group in the brompheniramine and O-H group in the 1-pentanol.

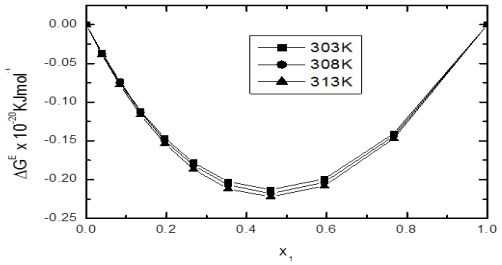

FIGURE 3. Excess Gibbs energy with concentration of brompheniramine.

It is noticed from figure 3, excess negative values increased up to in the molefraction 0.4600 then decreased while increasing mole fraction of brompheniramine. It confirm strength of hydrogen bonding is increased with mole fraction of brompheniramine and weakened with increasing the concentration of 1-pentanol.

CONCLUSION

Physical and acoustical parameters of bromphineramine and 1-pentanol were determined at 303,308 and 313K. Excess values and their sign suggested that hydrogen bonding interaction in the amine group present in the brompheniramine and hydroxyl group exists in the 1-pentanol.Ultrasonic velocity is noticed in the order of 303>308>313K.Decrease in ultrasonic velocity with increasing in temperature signifies that intermolecular force decreased due to increase in thermal energy of the selected liquid mixtures.

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