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Ultrasonic Studies of Brompheniramine with 1-Butanol at 303,308 and 313K

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ABSTRACT

The density (ρ), viscosity (η) and ultrasonic velocity (U) have been measured for the binary mixtures of Brompheniramine with 1-Butanol at 303,308 and 313K. From the experimental data, several acoustic parameters such as adiabatic compressibility (β), free length (L_f), free volume (V_f) , viscous relaxation time (τ) and Gibbs free energy (ΔG) have been calculated. The excess values of the above parameters (β^E, L_f^E, V_f^E ,τ^E and ΔG^E) were also determined and interpreted in terms of molecular association such as hydrogen bonding formed between the liquid mixtures. The results show that hetero association and homo association of molecules decrease with increase in the temperature.

Introduction

Ultrasonic velocity is fundamentally related with nature of the molecular interaction formed between the molecules present in the liquid mixture. Ultrasonic study is the simplest reliable technique to study the nature of molecular interaction of a binary or ternary liquid system. Such studies have great relevance in the pharmaceutical and chemical industries [1-5].Brompheniramine is used in the product of antihistamine drugs which is used in the treatment of common cold, allergic rhinitis. The molecular interaction studies of liquid mixtures with 1-butanol as one of the components is particular interest, since it is highly polar and self associated in pure state [6-8]. The survey of literature shows that no reports are recorded about the molecular interaction studies of the selected liquid system.

The present work is an attempt to elucidate the molecular interaction between brompheniramine with 1-butanol at 303,308 and 313K using ultrasonic technique.

Materials And Methods

Binary mixtures were prepared by mixing appropriate volume of the liquid components in the standard flasks with air tight caps. The masses were recorded on digital electronic balance (ACM-78094L,ACMAS Ltd,India) with an uncertainty of ±1mg.The density and viscosity have been measured by using specific gravity bottle and Ostwald's viscometer with accuracy ±0.01kgm^{-3} and ±0.001Nsm^{-2} respectively. The ultrasonic velocities in the liquid mixtures were measured by using a single crystal ultrasonic interferometer (Mittal Enterprizes,New Delhi Model:f81) operated at 2MHZ,which is calibrated with water. The accuracy in the ultrasonic velocity measurement is in the order of ±1ms^{-1}.All measurements are made using a constant temperature bath [INSREF model IRI-016C,India] by circulating water from the thermostat with accuracy ±0.01K. In this present study brompheniramine has been purchased from Varda Biotech Pvt.ltd, Mumbai, India.AR grade 1-butanol 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 the ultrasonic frequency and λ is ultrasonic wavelength.

Using the measured data, the following acoustic parameters were determined,

Adiabatic compressibility $\beta = \dfrac{1}{U^2\rho}$ (2)

Where U is the ultrasonic velocity and ρ is the 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 $V_f = \left[\dfrac{M_{eff}U}{\eta K}\right]^{3/2}$ (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 $\tau = \dfrac{4}{3}\beta\eta$ (5)

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

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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,

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

$A_{id} = x_1 A_1 + x_2 A_2$

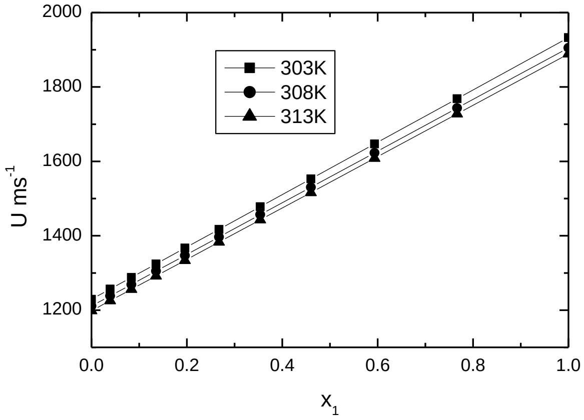
Here x_1 and x_2 are mole fractions of brompheniramine and 1-butanol respectively.A_1 and A_2 are acoustical parameters.

Result and Discussion

The experimentally determined, density (ρ), viscosity (η), ultrasonic velocity (U) and computed 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 n-methyl formate and 1-propanol at 303K,308K and 313K are presented in table 2.

It is observed from the table2, density (ρ) increased with increase in the concentration of brompheniramine. Moreover the temperature increased density of the liquid mixture decreased. The same trend is reflected in the viscosity measurements. It leads to notion that the system is more compact. Similar trend has been reported in propylene carbonate with n-alkanols [9].

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

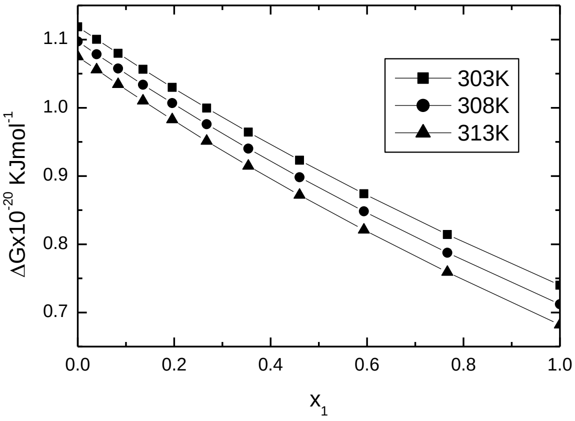


The increase in mole fraction of brompheniramine increases the net dispersive interactions and hence the ultrasonic velocity continuously increased as shown in the fig1.

It signifies that the temperature increased then the ultrasonic velocity decreased due to thermal agitation of the molecules present in the liquid system [10]. Adiabatic compressibility (β) is found to be decreased with increasing concentrations of brompheniramine with respect to the 1-butanol.This trend indicates that the specific interaction between the liquid mixtures. Similar trends have been obtained at various liquid mixtures.[11-15]

The decreasing trend of intermolecular free length (L_f) indicates the closer packing of the molecules in the liquid system. The same trend is noticed in the free volume (V_f),it confirms that the strong molecular interaction is formed through the hydrogen bonding interactions. The viscous relaxation time (τ) decreases with increasing the temperature and concentration of the brompheniramine .This trend may be due to loosening of cohesive force leading to breaking the structure of molecules.

Figure 2. Variation Gibbs free energy with brompheniramine



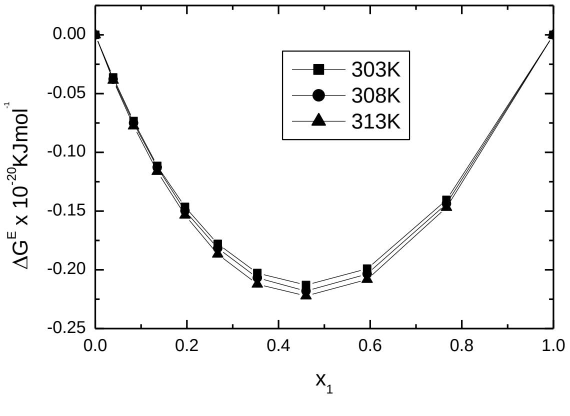
The reduction of free energy (ΔG) with temperature and the concentration of brompheniramine is as shown in the figure2.The curves signify that disassociation of the molecules in the liquid mixture.

In order to elucidate the molecular interaction between the liquid mixtures, it is of considerable interest to determine the excess parameter from the ideal mixing. 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.[16-18]

The 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.

In this present study, all the excess parameters show the negative excess values from the ideal mixing of components. This trend confirms the strong hydrogen boning interaction between the N-H group present in the brompheniramine and O-H group present in the 1-butanol.

Figure 3. Excess Gibbs energy with concentration of brompheniramine



It is observed from figure 3,the excess negative values increased up to in the molefraction 0.4600 after that decreased with increasing concentration of bromphen iramine.This change confirms that the hydrogen bonding interaction is increased in the concentration of brompheniramine and weakened with Increasing the concentration of 1-butanol.

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

X_1	ρ (Kgm^{-3})	η $\times 10^{-3}$ (Nsm^{-2})	U (ms^{-1})	β $\times 10^{-10}$ (m^2N^{-1})	L_f $\times 10^{-10}$ (m)	V_f $\times 10^{-8}$ (m^3mol^{-1})	τ $\times 10^{-12}$ (s)	ΔG $\times 10^{-20}$ ($KJmol^{-1}$)
T=303K								
0.0000	804.4	2.1508	1229.1	8.2291	0.5723	0.0985	2.3008	1.1187
0.0390	822.4	2.1988	1256.5	7.7017	0.5537	0.1181	2.2014	1.1003
0.0836	842.9	2.2537	1287.9	7.1525	0.5336	0.1420	2.0955	1.0797
0.1353	866.7	2.3173	1324.3	6.5789	0.5117	0.1715	1.9818	1.0563
0.1958	894.6	2.3918	1366.9	5.9827	0.4880	0.2082	1.8602	1.0299
0.2675	927.6	2.4800	1417.3	5.3668	0.4622	0.2547	1.7302	0.9996
0.3539	967.4	2.5863	1478.1	4.7313	0.4340	0.3148	1.5907	0.9644
0.4600	1016.3	2.7169	1552.8	4.0808	0.4030	0.3942	1.4413	0.9232
0.5936	1077.8	2.8813	1646.8	3.4212	0.3690	0.5023	1.2814	0.8740
0.7667	1157.5	3.0943	1768.6	2.7619	0.3316	0.6547	1.1110	0.8143
1.0000	1265.0	3.3814	1932.8	2.1161	0.2902	0.8803	0.9301	0.7400
T=308K								
0.0000	802.1	1.8643	1211.0	8.5012	0.5864	0.1193	2.0603	1.0972
0.0390	820.0	1.9060	1238.1	7.9556	0.5672	0.1431	1.9712	1.0784
0.0836	840.5	1.9537	1269.0	7.3882	0.5466	0.1721	1.8764	1.0575
0.1353	864.3	2.0089	1304.9	6.7948	0.5242	0.2078	1.7745	1.0338
0.1958	892.1	2.0736	1346.9	6.1789	0.4999	0.2523	1.6656	1.0068
0.2675	925.1	2.1502	1396.7	5.5412	0.4734	0.3087	1.5489	0.9760
0.3539	964.9	2.2426	1456.7	4.8840	0.4444	0.3815	1.4238	0.9402
0.4600	1013.7	2.3560	1530.4	4.2119	0.4127	0.4776	1.2900	0.8982
0.5936	1075.1	2.4988	1623.1	3.5307	0.3779	0.6085	1.1469	0.8482
0.7667	1154.7	2.6838	1743.3	2.8496	0.3395	0.7931	0.9942	0.7875
1.0000	1262.0	2.9332	1905.3	2.1828	0.2971	1.0665	0.8323	0.7120
T=313K								
0.0000	798.5	1.6302	1198.4	8.7201	0.5995	0.1436	1.8480	1.0750
0.0390	816.5	1.6669	1225.3	8.1575	0.5798	0.1723	1.7677	1.0558
0.0836	837.0	1.7089	1256.1	7.5722	0.5586	0.2071	1.6822	1.0344
0.1353	860.8	1.7575	1291.8	6.9615	0.5356	0.2501	1.5905	1.0102
0.1958	888.7	1.8144	1333.6	6.3269	0.5106	0.3037	1.4923	0.9827
0.2675	921.7	1.8819	1383.1	5.6715	0.4834	0.3715	1.3875	0.9512
0.3539	961.5	1.9632	1442.8	4.9961	0.4537	0.4591	1.2750	0.9147
0.4600	1010.3	2.0631	1516.0	4.3067	0.4213	0.5747	1.1550	0.8720
0.5936	1071.9	2.1888	1608.3	3.6067	0.3855	0.7321	1.0262	0.8209
0.7667	1151.6	2.3517	1727.8	2.9087	0.3462	0.9541	0.8892	0.7590
1.0000	1259.0	2.5712	1888.9	2.2261	0.3029	1.2827	0.7440	0.6820

Table 3. Excess parameters of brompheniramine with 1-butanol 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})	$\tau^E \times 10^{-12}$ (s)	ΔG^E $\times 10^{-21}$ ($KJmol^{-1}$)
T=303K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0390	-0.2890	-0.0760	-0.1089	-0.0459	-0.0363
0.0836	-0.5656	-0.1512	-0.2186	-0.0907	-0.0734
0.1353	-0.8231	-0.2243	-0.3278	-0.1335	-0.1116
0.1958	-1.0495	-0.2906	-0.4338	-0.1722	-0.1465
0.2675	-1.2271	-0.3464	-0.5293	-0.2039	-0.1780
0.3539	-1.3344	-0.3846	-0.6038	-0.2250	-0.2028
0.4600	-1.3363	-0.3953	-0.6393	-0.2289	-0.2130
0.5936	-1.1792	-0.3585	-0.6028	-0.2057	-0.1990
0.7667	-0.7804	-0.2441	-0.4321	-0.1388	-0.1405
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=308K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0390	-0.2992	-0.0792	-0.1314	-0.0412	-0.0378
0.0836	-0.5848	-0.1561	-0.2639	-0.0812	-0.0750
0.1353	-0.8515	-0.2306	-0.3966	-0.1196	-0.1128
0.1958	-1.0852	-0.2986	-0.5246	-0.1542	-0.1498
0.2675	-1.2698	-0.3561	-0.6398	-0.1829	-0.1816
0.3539	-1.3811	-0.3962	-0.7301	-0.2019	-0.2068
0.4600	-1.3828	-0.4062	-0.7741	-0.2054	-0.2181
0.5936	-1.2199	-0.3677	-0.7306	-0.1844	-0.2035
0.7667	-0.8073	-0.2509	-0.5242	-0.1245	-0.1437
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=313K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0390	-0.3093	-0.0813	-0.1572	-0.0372	-0.0387
0.0836	-0.6050	-0.1610	-0.3173	-0.0735	-0.0775
0.1353	-0.8800	-0.2377	-0.4762	-0.1081	-0.1163
0.1958	-1.1217	-0.3083	-0.6294	-0.1395	-0.1535
0.2675	-1.3115	-0.3676	-0.7681	-0.1652	-0.1867
0.3539	-1.4258	-0.4083	-0.8763	-0.1823	-0.2122
0.4600	-1.4262	-0.4176	-0.9289	-0.1852	-0.2222
0.5936	-1.2586	-0.3794	-0.8767	-0.1665	-0.2082
0.7667	-0.8325	-0.2590	-0.6285	-0.1124	-0.1469
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Conclusion

The physical and acoustical parameters were determined in the binary mixture of Bromphineramine and 1-butanol at 303,308 and 313K.The calculated excess values and their sign signify that the specific hydrogen bonding formed in the amine group of the brompheniramine and hydroxyl group present in the 1-bitanol.Moreover ultrasonic velocity is in the order of 303>308>313K.The decrease in velocity with increase in temperature at any concentration signifies that decrease in intermolecular forces due to increase in thermal energy of the liquid system.

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