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Mathematical Analysis of Intermolecular Interaction Studies Between Brompheniramine and 1-Hexanol at Various Temperatures Using Ultrasonic Velocity.

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ABSTRACT

Viscosity (η), density (ρ), and ultrasonic velocity (U), of brompheniramine with 1-hexanol were determined at 303K , 308K and 313K.From the experimental observations, adiabatic compressibility (β), viscous relaxation time (τ), free volume (V_f), free length (L_f), and Gibbs free energy (ΔG) were calculated. Deviations of that parameters (β^E, L_f^E, V_f^E,τ^E and ΔG^E) with ideal values were analyzed using mathematical relations and fitted with Redlich Kister polynomial equations. Standard deviations of the determined values of various parameters were calculated. From the observations, temperature takes a vital role and dissociation take place in the increasing temperature.

Introduction

The ideal values of various physico chemical quantities such as viscosity, density, ultrasonic velocity vary with solute and solvent interactions. Formation of bonding with functional groups takes a vital role in those parameters changes with pure liquids [1]. More over the sign and magnitude of the variation signifies the strength of the intermolecular interaction between the selected liquid compounds. In order to support the findings, derived quantities like adiabatic compressibility, viscous relaxation time, free volume, free length and Gibb's free energy were calculated [2]. Brompheniramine is one of the pharmaceutical important amine group compounds. It is effectively used in allergic rhinitis and common cold. Self association and polar nature of alcohol leads to the interactions between the amine and hydroxyl group of the liquid mixtures. Temperature variations provide the significant variations in the strength of interactions. Redlich Kister polynomial and standard deviations were used mathematically to determine the errors in the measurements.

Materials and methods

Binary mixtures of brompheniramine and 1-hexanol were prepared in different concentrations using mole fraction. In order to avoid the moisture and minimize the errors, the mixture was kept in standard flasks with firmly air tight caps. Digital electronic balance (ACM-78094L,ACMAS Ltd, India) was used to measure the mass of the mixture with accuracy of ±1mg. Specific gravity bottle was used to determine the relative density of the compounds with double distilled water as a standard with accuracy ±0.01kgm^{-3} and Ostwald's viscometer with accuracy ±0.001Nsm^{-2} was used in the measurement of viscosity of the solution. An ultrasonic interferometer of 2MHz which was produced by a single crystal (Mittal Enterprizes,New Delhi Model:f81) with accuracy ±1ms^{-1} was used to measured the ultrasonic velocity in the system. Liquid system was maintained in a constant temperature bath [INSREF model IRI-016C, India] with accuracy ±0.01K. Analytical grade of brompheniramine and 1-hexanol was used with standard purification methods.

Theory

Various physicochemical parameters were determined as listed below,

$$\text{Ultrasonic velocity } (U) = f\lambda \quad (1)$$

Here f is ultrasonic frequency and λ is ultrasonic wavelength.

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

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

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

Where K_T is the temperature dependent constant.

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

Where M_{eff} is the effective molecular weight ($M_{eff}=m_1x_1+m_2x_2$) m 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.

$$\text{Viscous relaxation time } (\tau) = \frac{4}{3}\beta\eta \quad (5)$$

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

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

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

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

$A_{id}=x_1 A_1+x_2A_2$

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

The excess parameters were fitted with the Redlich Kister polynomial equation as follow,

$$\Delta A = x_1x_2\left[a_0 + a_1\left(x_1 - x_2\right) + a_2\left(x_1 - x_2\right)\right] \quad (8)$$

$$\text{Standard deviation } (\sigma) = \left[\frac{\Sigma\left(X_{\exp} - X_{cal}\right)^2}{N-n}\right]^{1/2} \quad (9)$$

Results and discussion

The determined physicochemical parameters were listed in table-1. While increasing the concentration of 1-hexanol, packing of molecules weakened. It leads to the decreasing density (ρ) with the increasing 1-hexanol concentration. Similar variations were observed in the viscosity (η) of the liquid mixture. Steric effect also takes a key role in the decreasing viscosity [3]. Moreover the increasing concentration of 1-hexanol with respect to brompheniramine, the cohesive force acting between the brompheniramine and 1-hexanol is weakened.[4-6].The change in ultrasonic velocity(U) in a medium related with the variation of intermolecular free length due to solute and solvent present in the liquid mixtures. The ultrasonic velocity decreased with the increasing concentration of 1-hexanol for the entire selected range of temperature. It leads to form hydrogen bonding between the corresponding functional groups exist in the liquid mixtures [7]. Now free length (L_f) decreased with brompheniramine concentrations is as listed in the table2. This effect is due to structural changes in the liquid mixtures.

As the temperature increased, ultrasonic velocities decreased as shown in the fig (1). It signifies dissociation takes place with temperature and concentration of alcohol [8]. Adiabatic compressibility (β) was increased with the 1-hexanol. Internal pressure increased with the same trend against the free volume. It signifies that the liquid mixtures were in a more compact state. Acoustic impedance variation signifies the inertial and elastic properties of a system. Acoustic impedance (Z) increased with brompheniramine concentration. It supports the hydrogen bonding formation between the brompheniramine with 1-hexanol. Relaxation time (τ) increased with the concentration of brompheniramine and temperature. The change observed fig (2) in Gibb's free energy (ΔG) with 1-hexanol concentrations in the entire temperature range support the weak hydrogen bonding present in the liquid system. It may be (i) Free volume difference observed in the dissimilar molecules.(ii) Contraction between brompheniramine and 1-hexanol through N-H---O-H and (iii)Specific interactions present in the alcohol and brompheniramine. The change in sign and magnitude of the excess parameters with ideal value based on the strength of intermolecular interaction existing in the selected system. The change in excess parameters values were listed in table2.Moreover variation of V^E due to the two types of interactions in the system: (i) Dispersion forces or weak dipole-dipole leads to a positive changes,(ii) Negative sign may due to specific interactions, charge transfer and hydrogen bond formation [9-10]. All the excess parameters vales were observed in the system at the three temperatures. More negative deviation observed with brompheniramine concentration and temperature. It reveals that the intermolecular interaction decreased with increase in the temperature. The variation of ΔG^E is as plotted in fig(3). It was observed as of 303K<308K<313K. It may due to rupture of hydrogen bonding formed in 1-hexanol with brompheniramine.

Table 1. Physico chemical parameters of brompheniramine with 1-hexanol at various temperatures

X_1	ρ(kgm^{-3})	$\eta\times 10^{-3}$(Nsm^{-2})	U (ms^{-1})	$\beta\times10^{-10}$ (m^{2}N^{-1})	$L_f\times10^{-11}$ (m)	$V_f\times 10^{-8}$ m^{3}mol^{-1})	$\tau\times 10^{-12}$ (s)	$\Delta G\times 10^{-20}$ KJmol^{-1})
T=303K								
0.0000	803.2	1.9747	1228	8.2588	5.7341	0.2220	2.1745	1.0708
0.0311	821.2	2.0227	1255	7.7290	5.5471	0.2416	2.0844	1.0524
0.0757	841.7	2.0776	1287	7.1772	5.3454	0.2655	1.9881	1.0318
0.1274	865.5	2.1412	1323	6.6010	5.1264	0.295	1.8845	1.0084
0.1879	893.4	2.2157	1366	6.0021	4.8883	0.3317	1.7732	0.9820
0.2596	926.4	2.3039	1416	5.3836	4.6296	0.3782	1.6537	0.9517
0.3460	966.2	2.4102	1477	4.7455	4.3466	0.4383	1.5250	0.9165
0.4521	1015.1	2.5408	1552	4.0924	4.0364	0.5177	1.3864	0.8753
0.5857	1076.6	2.7052	1646	3.4304	3.6955	0.6258	1.2373	0.8261
0.7588	1156.3	2.9182	1767	2.7689	3.3201	0.7782	1.0773	0.7664
1.0000	1263.8	3.2053	1932	2.1209	2.9058	1.0038	0.9064	0.6921
T=308K								
0.0000	800.9	1.6882	1210	8.5323	5.8747	0.2428	1.9205	1.04931
0.0311	818.8	1.7299	1237	7.9840	5.6828	0.2666	1.8415	1.03051
0.0757	839.3	1.7776	1268	7.4139	5.4762	0.2956	1.7572	1.00961
0.1274	863.1	1.8328	1304	6.8178	5.2514	0.3313	1.6661	0.98591
0.1879	890.9	1.8975	1346	6.1992	5.0075	0.3758	1.5684	0.95891
0.2596	923.9	1.9741	1395	5.5582	4.7418	0.4322	1.4631	0.92811
0.3460	963.7	2.0665	1455	4.8988	4.4514	0.5050	1.3497	0.89231
0.4521	1012.5	2.1799	1529	4.2240	4.1335	0.6011	1.2277	0.85031
0.5857	1073.9	2.3227	1622	3.5403	3.7841	0.7320	1.0964	0.80031
0.7588	1153.5	2.5077	1742	2.8568	3.3993	0.9166	0.9552	0.73961
1.0000	1260.8	2.7571	1904	2.1878	2.9748	1.1900	0.8042	0.66411
T=313K								
0.0000	797.3	1.4541	1197	8.7522	6.0061	0.2671	1.6968	1.0271
0.0311	815.3	1.4908	1224	8.1869	5.8089	0.2958	1.6273	1.0079
0.0757	835.8	1.5328	1255	7.5988	5.5964	0.3306	1.553	0.9865
0.1274	859.6	1.5814	1291	6.9853	5.3657	0.3736	1.4728	0.9623
0.1879	887.5	1.6383	1332	6.3478	5.1150	0.4272	1.3866	0.9348
0.2596	920.5	1.7058	1382	5.6896	4.8425	0.495	1.2940	0.9033
0.3460	960.3	1.7871	1442	5.0114	4.5448	0.5826	1.1941	0.8668
0.4521	1009.1	1.8870	1515	4.3192	4.2193	0.6982	1.0867	0.8241
0.5857	1070.7	2.0127	1607	3.6166	3.8608	0.8556	0.9705	0.7730
0.7588	1150.4	2.1756	1727	2.9162	3.4669	1.0776	0.8459	0.7111
1.0000	1257.8	2.3951	1888	2.2313	3.0326	1.4062	0.7125	0.6341

Table 2.Excess parameters of brompheniramine with 1-hexanol at various temperatures

x_1	$\beta^E \times 10^{-10}$ (m^2N^{-1})	$L_f^E \times 10^{-11}$ (m)	$V_f^E \times 10^{-8}$ (m^3mol^{-1})	$\tau^E \times 10^{-12}$ (s)	$\Delta G^E \times 10^{-21}$ ($KJmol^{-1}$)
T=303K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0311	-0.2890	-0.0760	-0.1089	-0.0459	-0.0363
0.0757	-0.5656	-0.1512	-0.2186	-0.0907	-0.0734
0.1274	-0.8231	-0.2243	-0.3278	-0.1335	-0.1116
0.1879	-1.0495	-0.2906	-0.4338	-0.1722	-0.1465
0.2596	-1.2271	-0.3464	-0.5293	-0.2039	-0.178
0.3460	-1.3344	-0.3846	-0.6038	-0.2250	-0.2028
0.4521	-1.3363	-0.3953	-0.6393	-0.2289	-0.2130
0.5857	-1.1792	-0.3585	-0.6028	-0.2057	-0.199
0.7588	-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
0.0311	-0.2992	-0.0792	-0.1314	-0.0412	-0.0378
0.0757	-0.5848	-0.1561	-0.2639	-0.0812	-0.0750
0.1274	-0.8515	-0.2306	-0.3966	-0.1196	-0.1128
0.1879	-1.0852	-0.2986	-0.5246	-0.1542	-0.1498
0.2596	-1.2698	-0.3561	-0.6398	-0.1829	-0.1816
0.3460	-1.3811	-0.3962	-0.7301	-0.2019	-0.2068
0.4521	-1.3828	-0.4062	-0.7741	-0.2054	-0.2181
0.5857	-1.2199	-0.3677	-0.7306	-0.1844	-0.2035
0.7588	-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
0.0311	-0.3093	-0.0813	-0.1572	-0.0372	-0.0387
0.0757	-0.6050	-0.1610	-0.3173	-0.0735	-0.0775
0.1274	-0.8800	-0.2377	-0.4762	-0.1081	-0.1163
0.1879	-1.1217	-0.3083	-0.6294	-0.1395	-0.1535
0.2596	-1.3115	-0.3676	-0.7681	-0.1652	-0.1867
0.3460	-1.4258	-0.4083	-0.8763	-0.1823	-0.2122
0.4521	-1.4262	-0.4176	-0.9289	-0.1852	-0.2222
0.5857	-1.2586	-0.3794	-0.8767	-0.1665	-0.2082
0.7588	-0.8325	-0.2590	-0.6285	-0.1124	-0.1469
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 3 . Redlich-Kister coefficients and standard deviations of brompheniramine and 1-hexanol at various temperature

Parameters	Temperature (K)	a_0	a_1	a_2	σ
β^E $\times 10^{-10}$ (m^2N^{-1})	303	-0.348	-0.443	-0.0986	0.004
	308	-0.218	-0.197	0.019	0.004
	313	-0.218	0.517	0.012	0.004
L_f^E $\times 10^{-11}$ (m)	303	-0.904	0.596	0.295	0.016
	308	-0.666	0.292	0.317	0.003
	313	-1.064	0.635	0.423	0.017
V_f^E $\times 10^{-8}$ (m^3mol^{-1})	303	-0.149	-0.510	0.657	0.005
	308	-0.203	-0.890	1.088	0.011
	313	-0.235	-1.348	1.512	0.019
τ^E $\times 10^{-12}$ (s)	303	-1.928	1.235	0.685	0.009
	308	0.188	0.553	-0.741	0.002
	313	0.438	-2.031	-2.309	0.016
ΔG^E $\times 10^{-20}$ ($KJmol^{-1}$)	303	0.206	0.480	-0.687	0.005
	308	0.948	0.973	-1.915	0.013
	313	1.817	1.633	-3.343	0.012

Redlich Kister polynomial coefficient and the corresponding standard deviation values of the physic chemical parameters were listed in table 3.The standard deviation values were very small. The validity of the experimental and mathematically derived values of the parameters was correlated. The significant variation obtained in the physicochemical parameters suggested that hydrogen bonding strength between 1-hexanol and brompheniramine was in the order of 303K <308K < 313K

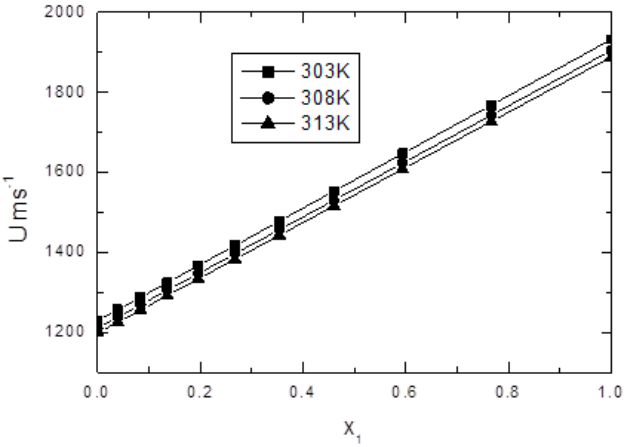

Fig 1. Variation in ultrasonic velocity with mole fraction of brompheniramine with 1-hexanol at 303K,308K and 313K

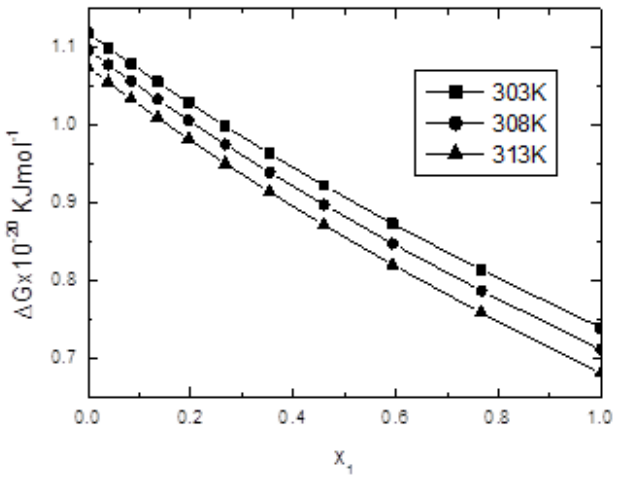

Fig 2. Variation in Gibbs free energy with mole fraction of brompheniramine with 1-hexanol at 303K, 308K and 313K.

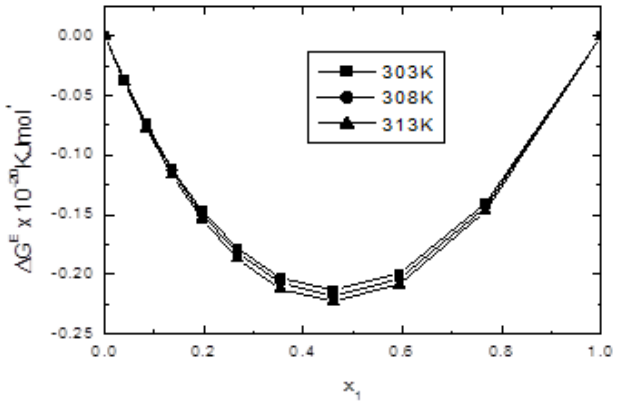

Fig 3. Variation in excess Gibbs free energy with mole fraction of brompheniramine with 1-hexanol at 303K, 308K and 313K

Conclusions

The viscosity, density and ultrasonic velocity were experimentally determined. Based on the experimental data, adiabatic compressibility, free length and internal pressure were mathematically derived. The excess values of those parameters with ideal values were also calculated. The significant variations in the parameters were analyzed insight of the complex formation between the liquid mixtures. The decreasing ultrasonic velocity and change in the sign and magnitude of excess parameters suggested that the brompheniramine concentrations and increase in the temperature leads the dissociation of hydrogen bonding which formed between 1-hexanol in brompheniramine mixture at various temperatures. Thus the intermolecular interaction of 1-hexanol with brompheniramine was in the trend of 303K < 308K< 313K.

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