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ULTRASONIC BEHAVIOUR OF AQUEOUS SODIUM SALT OF ETHYLPARABEN WITH ETHYLENE GLYCOL AND PROPYLENE GLYCOL AT 298.15 K TEMPERATURE

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Abstract

The acoustical parameters such as acoustic impedance, intermolecular free length, adiabatic compressibility, relative association and Gibb's free energy of EG and PG with sodium ethylparaben have been studied at 298.15K from ultrasonic velocity and density measurement. The acoustic impedance shows the opposite trend with the other various computed parameters but on the other hand, adiabatic compressibility and intermolecular free length follow the similar pattern. The presence of sturdy associations exists among the solute and solvent molecules in the present system investigated. The glycols i.e. EG and PG forms the structure in the water. PG> EG is the trend followed by structure forming tendency of glycols.
Keywords: ultrasonic velocity, relative association, density.

Introduction

The travelling of ultrasonic waves in liquid is a very useful technique used by researcher to explore the properties of liquid. One can study the physical and chemical properties of solution and its molecular interaction by estimating density, viscosity and ultrasonic speed. Through literature survey it is found that the ultrasonic study is very beneficial to understand the behavior and strength of interactions between the molecules in the binary or ternary mixtures (Aswale *et al*., 2012; Kumar *et al*., 2015; Ali *et al*., 1999; Kumar *et al*., 2014). Due to simplicity and accuracy of the ultrasonic technique it is being most widely used in the study of liquid state among the three states of matters (Sheba *et al*., 2014; Kumar *et al*., 2016). The study of various types of fragmental interactions among solute and solvent is of vast interest in various branches of physics and chemistry that help us to know whether solute disrupts or modifies the solvent (Kulkarni *et al*., 2016; Kumar *et al*., 2016). Ethylene glycols are solvents that constitute two hydroxyl members in each atom in which inter and intra sub-atomic hydrogen bonds were arranged between –O- and –OH groups (Kaur *et al*., 2017). Ethylene glycols with the general formula $H(OCH_2CH_2)_nOH$, where *n* is from 1–5 termed as the series of synthetic linear oligomers of escalating oxyethylene units each molecule (Fowles *et al*., 2017). The researchers have got widely interested in examining the study of glycols (Sharma *et al*., 2018; Sonika *et al*., 2018; Kaur *et al*., 2018). Parabens are defined to be the class of extremely consumed preservatives in cosmetics and pharmaceutical materials (Thakur *et al*., 2019; Thakur *et al*., 2019; Thakur *et al*., 2020; Thakur *et al*., 2020).In order to determine the behaviour of molecular interaction existing in the studied system, the ultrasonic technique has been extremely utilized (Chakraboratry *et al*., 2020; Chakrabortary *et al*., 2019; Sharma *et al*., 2018; Vasantharani *et al*., 2009; Pal *et al*., 2013). The parameter partial molar volume is being considered as helpful tool in order to determine the different interactions in water and waterless solutions (Thakur *et al*., 2015; Thakur *et al*., 2014; Thakur *et al*., 2014; Thakur *et al*., 2015; Thakur *et al*., 2016 Sharma *et al*.,2018). For identifying the structural characteristics of system mixture the volumetric as well as viscometric behaviour is being considered (Ali *et al*., 2002; Oswal, *et al*., 2000; Rawat *et al*., 2008; Peralta *et al*., 2002; Naidu *et al*., 2003 Saravanakumar *et al*., 2012). At 298.15K the data of density and ultrasonic velocity for EG and PG with SEP in water medium has been measured. The measured parameters are used in order to evaluate the various acoustical parameters and the prediction is based upon the fragmental interactions in the current system examined. There may be existence of different types of interaction on the mixing of solvent. The magnitude of forces depends upon the type of solvent used and it decreases or increases accordingly. In the mixing components it is found that bond breaking or breaking of liquid order predominates over other types of molecular interactions. The ultrasonic velocity (c) and density (ρ) were used to calculate the parameters such as free adiabatic compressibility, acoustic impedance, intermolecular

free length, relative strength, Gibb's free energy. The trends of these acoustical parameters have the ability to reveal the nature and behavior of a system more precisely.

Chemicals and Technique

Chemicals

The chemicals utilized in the current study are taken from Loba chemie Pvt. Ltd. India. Sodium ethylparaben and both glycols of 99% AR grade has been used in the studied system. Anton Paar DSA 5000 M density and velocity meter is used to make ultrasonic velocity and density measurement. For graphical representation ORIGIN software is utilized. The Values of ultrasonic velocity and density were used to calculate the parameters like as free adiabatic compressibility, acoustic impedance, intermolecular free length, relative strength, Gibb's free energy.

Methods

The intermolecular free length, acoustical impedance, adiabatic compressibility, relative strength, Gibb's free energy and relative association are computed from these formulas:

Acoustic impedance

Acoustic impedance is the resistance offered to the propagation of ultrasonic wave in the medium and can be defined as the product of density (ρ) of the medium and ultrasonic velocity (U) of the same medium. It can be written as

$$Z = \rho \times U$$

Adiabatic compressibility

Adiabatic compressibility is fractional reduction in volume per unit increase of pressure, when no heat flows in or out. This variation is related to the compressibility in a medium by thermodynamic relation:

$$\beta = (1/V)\ (dV/\ dP)$$

Adiabatic compressibility can also be calculated from the ultrasonic velocity (c) and density (ρ) of the medium using equation:

$$\beta = 1/\ (c^2 \times \rho)$$

Intermolecular free length

In 1952, Jacobson suggested an empirical relation for calculating the intermolecular free length of liquids. [8] According to the studies, L_f is given by:

$$L_f = K_T \times \beta^{1/2}$$

Where, K_T = Jacobson constant whose value is 2.0965×10^{-6}

β = compressibility of the liquid.

Intermolecular free length can also be expressed in terms of ultrasonic velocity and density as:

$$L_f = K/\ (c \times \rho^{1/2})$$

Where, c = ultrasonic velocity of experimental liquid

ρ = density of liquid of experimental liquid.

Relative strength

$$r = 1\text{-}[U/U_\infty]$$

Relative association

$$R_A = (\rho/\rho_0)/(U_0/U)^{1/3}$$

Gibb's Free Energy

It is the energy associated with chemical reaction that can be used to do work. The change in this energy can be calculated as

$$\Delta G = K_B\, T \ln (KB\ T\ \tau/\ h)$$

Where, K_B = Boltzmann's constant whose value is 1.38×10^{-23}

T = absolute temperature (295 K)

τ = relaxation time

h = Planck's constant having value 6.634×10^{-34}.

Result and Discussion

The acoustical velocity and density of SEP with Eg and PG in water medium at 298.15K temperature is obtained from our previous work (Thakur *et al.,* 2020). The different acoustical parameters such as impedance, adiabatic compressibility, Gibb's free energy, intermolecular free length and relative association are evaluated and are indexed in Table 1.

The presence of sturdy association amid liquid system has been predicted from linearly varying acoustic impedance w.r.t. concentration. The penetration and reflection of acoustical waves is afflicted by this specific factor in mixture. The acoustic impedance escalates from EG to PG with the concentration suggesting the fragments of PG are highly attracted in comparison to EG.

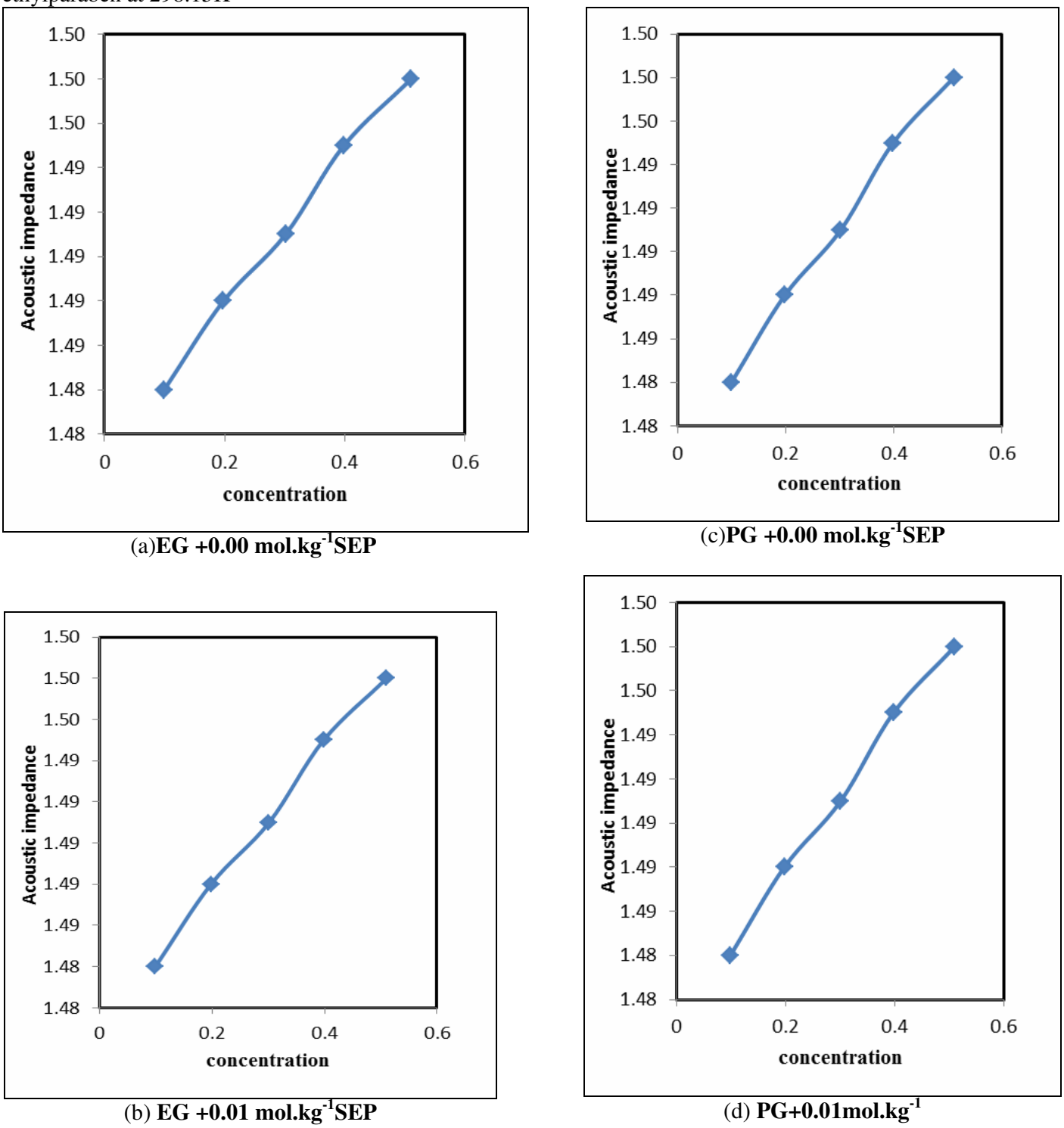
The value depicted in Table 1 of adiabatic compressibility decreases w.r.t. increase in the solute quantity as well as with SEP quantity which further tells that the studied liquid mixtures fragments are strongly attached together. There is the presence of strong bonding of PG molecules as compared to EG molecules. Therefore the ultrasonic velocity data is showing opposite trend w.r.t. to adiabatic compressibility hence, justifying the expression.

The value of intermolecular free length w.r.t. concentration is listed in Table 1. There is decrease in the value of intermolecular free length decreases with rise in sodium ethylparaben and glycols quantity. The adiabatic compressibility and intermolecular free length displays similar trend as depicted by their mathematical expression which is in agreement with experimental results.

Table 1: Computed Values of Acoustic impedance (Z), Adiabatic compressibility (β), Intermolecular free length (L_f) for ternary liquid mixture at 298.15K

(*m*) Glycols	**Concentration**	**Impedance (Z) kg m^{-2} s^{-1} × 10^5**	**Adiabatic compressibility (β) N/m^2 × 10^{-7}**	**Intermolecular free length (L_f) Å x 10^{-10}**
(0.00) EG	0.0000	1.479	4.561	91.41
	0.0996	1.483	4.539	91.19
	0.2010	1.488	4.518	90.97
	0.2991	1.492	4.496	90.76
	0.3938	1.496	4.475	90.54
	0.4972	1.500	4.454	90.33
(0.01) EG	0.0000	1.484	4.534	91.13
	0.1117	1.488	4.512	90.91
	0.1995	1.491	4.497	90.76
	0.2957	1.495	4.476	90.55
	0.3972	1.499	4.461	90.40
	0.4939	1.503	4.440	90.18
(0.00) PG	0.0000	1.479	4.561	91.41
	0.0992	1.484	4.536	91.15
	0.1980	1.488	4.510	90.89
	0.3014	1.491	4.491	90.70
	0.3983	1.495	4.472	90.51
	0.5106	1.498	4.453	90.32
(0.01) PG	0.0000	1.484	4.534	91.13
	0.1011	1.488	4.515	90.94
	0.1998	1.492	4.489	90.68
	0.3009	1.497	4.458	90.37
	0.3977	1.502	4.434	90.12
	0.4943	1.507	4.403	89.81

Figure 1 The variation of acoustic impedance with respect to concentration for EG and PG in aqueous sodium ethylparaben at 298.15K



(a)**EG +0.00 mol.kg^{-1}SEP**

(c)**PG +0.00 mol.kg^{-1}SEP**

(b) **EG +0.01 mol.kg^{-1}SEP**

(d) **PG+0.01mol.kg^{-1}**

Figure 1. Variation of Acoustic impedance with respect to various EG and PG concentration

Table 2: Computed Values of Gibbs free energy (ΔG) and Relative association (R_A) for ternary liquid mixture at 298.15K

(*m*) Glycols	Concentration	Gibb's free energy (ΔG) KJ mol^{-1} × 10^{-20}	Relative association (R_A)
(0.00) EG	0.0000	1.2369	1.0020
	0.0996	1.2373	1.0048
	0.2010	1.2380	1.0076
	0.2991	1.2380	1.0103
	0.3938	1.2384	1.0130
	0.4972	1.2385	1.0135

(0.01) EG	0.0000	1.2570	1.0010
	0.1117	1.2575	1.0042
	0.1995	1.2568	1.0068
	0.2957	1.2586	1.0089
	0.3972	1.2589	1.0116
	0.4939	1.2593	1.0220
(0.00) PG	0.0000	1.2775	1.0027
	0.0992	1.2781	1.0057
	0.1980	1.2787	1.0079
	0.3014	1.2792	1.0102
	0.3983	1.2797	1.1232
	0.5106	1.2802	1.1376
(0.01) PG	0.0000	1.2979	1.0000
	0.1011	1.2987	1.0029
	0.1998	1.2990	1.0065
	0.3009	1.2997	1.0095
	0.3977	1.3002	1.0131
	0.4943	1.3005	1.0234

Table 2 : Shows the data of Gibb's free energy

The energy related to utilization of work is provided by The Gibb's free energy It can be found from the data that the value of Gibb's free energy is increasing with increase in the concentration of solute.

The relative association shows the linear trend with concentration. The data of relative association escalates with concentration increase. The relative association elevates by elevation in the quantity of glycols i.e. from EG to PG. From the closest data of relative association, it has been found that the examined ternary liquid mixture is essentially ideal in nature.

Conclusion

The data of ultrasonic velocity shows the sturdy fragment associations amid investigated system of glycols with sodium ethylparaben in water medium. With decrease in intermolecular free length the data of ultrasonic velocity rises with rise in the quantity of EG and PG and SEP. Acoustic impedance, relaxation time, and relative association elevates with elevation in the concentration of glycols. There is linear variation of acoustical parameters w.r.t. concentration predicting there is no development of complex in the mixture or system.

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