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Karbala International Journal of Modern Science xx (2018) 1–8
http://www.journals.elsevier.com/karbala-international-journal-of-modern-science/

Theoretical assessment of ultrasonic velocities of binary liquid mixtures containing p-chloroacetophenone with 1-alcohols at temperatures from 303.15 K to 318.15 K

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Received 30 August 2017; revised 12 December 2017; accepted 13 December 2017

Abstract

Ultrasonic velocities and densities and viscosities of parachloroacetophenone with alcohols have been measured at temperatures range from 303.15 K to 318.15 K over the entire composition range of mole fraction. Theoretical ultrasonic velocities were correlated by using Nomoto's relation (U_{NOM}), Impedance relation (U_{IR}), Ideal mixing relation (U_{IMR}), Junjie's relation (U_J) and Rao's specific velocity (U_R). The theoretical and experimental values found good agreement with molecular interaction parameter (α) and chi square Goodness-of-fit test (X^2).

Keywords: Molecular interaction parameter; Chi square test; Theoretical velocities; Ultrasonic velocity

1. Introduction

The ultrasonic velocity and density are vital parameters used in understanding the nature of molecular association emanating from intermolecular interactions between liquid components mixtures. The experimental and theoretical values of ultrasonic velocities in binary liquid mixtures show deviations [1,2]. The interpretation of ultrasonic velocities has been widely useful for understanding the molecular interactions between polar and non-polar groups between component molecules [3]. Similar kind of research work has been done by earlier workers. In the present paper, the theoretical ultrasonic velocities of binary liquid mixtures containing Parachloroacetophenone (PclAp) and 1-Alcohols (1-Propanol, 1-Butanol, 1-Pentanol) over the entire mole fraction range and temperatures from 303.15 K to 318.15 K have been correlated with Nomoto [4], Van Dael and Vangeel ideal mixing relations [5], impedance relation [6], junjie [7], and Rao's specific velocity [8]. Proper applicability of the theories of present work has been discussed. The results were evaluated in terms of molecular interaction parameter (α) and chi square Goodness-of-fit test (X^2). The deviation of molecular interaction parameter from unity has also been calculated for explaining the non-ideality in the liquid mixtures.

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Peer review under responsibility of University of Kerbala.

https://doi.org/10.1016/j.kijoms.2017.12.003

2. Materials and methods

Parachloroacetophenone (pclAp), is taken as the main component and 1-Alcohols (1-Propanol, 1-Butanol, 1-Pentanol) are taken as secondary components as three binary systems. These chemicals purchased from S.D. Fine chemicals Ltd, India are used in the present work. The selected solvents were purified by adopting the methods as described in the literature [13,14]. The mixtures were prepared by mixing weighed amounts of the pure liquids by adopting the method of a closed system by using Mettler Toledo (ME204) balance with the precision of ±0.1 mg. Mixtures were allowed to stand for some time before every measurement so as to avoid air bubbles. Ultrasonic velocities (u) and densities were determined by using an Ultrasonic Interferometer Model DSA-5000M, from Anton Paar India Pvt. Ltd. The densities were measured by taking the sample of 2 ml.

3. Theory

Explanation and evaluation of various ultrasonic theories are as follows:

(1) **Nomoto theory**

It is based on the additivity of molar sound velocity(R) and no volume change on mixing.

$$R = M/\rho U^2 \tag{1}$$

Where U and ρ are ultrasonic velocity and density which are evaluated experimentally. M is the mean molecular weight

$$M = (X_1M_1 + X_2M_2) \tag{2}$$

Where M_1 and M_2 are the molecular weights of constituent components

$$U_{Nom} = \left[\frac{X_1R_1 + X_2R_2}{X_1V_1 + X_2V_2}\right]^3 \tag{3}$$

X_1 and X_2 are the mole fractions of 1st and 2nd components. V_i is the molar volume of component i. R_1 and R_2 are the molar sound velocity of 1st and 2nd components.

(2) **Impedance relation**

The specific acoustic impedance relation is used for evaluating the ultrasonic velocity in the liquid mixtures

$$U_{IR} = \Sigma X_i Z_i / \Sigma X_i \rho_i \tag{4}$$

Where X_i is the mole fraction, ρ_i is the density of the mixture, Z_i is the acoustic impedance.

(3) **Junjie equation**

This equation is given by Junjie, which depends on mole fraction, molecular weight and density of the mixture is given as

$$U_J = \left(\frac{X_1M_1}{\rho_1} + \frac{X_2M_2}{\rho_2}\right) \Bigg/ \left[\{X_1M_1 + X_2M_2\}^{1/2}\left\{\frac{X_1M_1}{\rho_1 U_1^2} + \frac{X_2M_2}{\rho_2 U_2^2}\right\}\right]^{1/2} \tag{5}$$

(4) **Rao's specific velocity relation**

Rao's specific velocity relation is the ratio of molar sound velocity or Rao's constant (R) and molar volume (V)

$$U_R = \left(\frac{R}{V}\right)^3 \tag{6}$$

(5) **Ideal mixing relation**

Van Dael and Vangeel suggested the ideal mixing relation

$$\frac{1}{X_1M_1 + X_2M_2}\frac{1}{U_{imr}^2} = \frac{X_1}{M_1U_1^2} + \frac{X_2}{M_2U_2^2} \tag{7}$$

Where U_{imr} is the ideal mixing relation of ultrasonic velocity, U_1 and U_2 are the velocities of the individual components.

(6) **Molecular interaction parameter (α) is given by**

$$\alpha = \left(U_{exp}^2 \Big/ U_{imr}^2\right) - 1 \tag{8}$$

Please cite this article in press as: R.S. Maganti et al., Theoretical assessment of ultrasonic velocities of binary liquid mixtures containing p-chloroacetophenone with 1-alcohols at temperatures from 303.15 K to 318.15 K, Karbala International Journal of Modern Science (2018), https://doi.org/10.1016/j.kijoms.2017.12.003