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Acoustic, volumetric, transport and spectral studies of binary mixtures of 1-tert-butoxy-2-propanol with alcohols at different temperatures

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ABSTRACT

The molecular interactions have been studied in the binary mixtures of 1-tert-butoxy-2-propanol $(CH_3)_3COCH_2CH(OH)CH_3$ with four structurally different alcohols, viz., 1-propanol $CH_3(CH_2)_2OH$, 2-propanol $(CH_3)_2CHOH$, 1-butanol $CH_3(CH_2)_3OH$ and 2-butanol $CH_3CH_2CH(OH)CH_3$, through the behavior of measured densities, ρ, speeds of sound, u at 293.15, 298.15, 303.15, 308.15 and 313.15 K and viscosities, η at 298.15, 303.15 and 308.15 K. The experimental data were used to calculate the excess molar volumes, V_m^E, excess molar isentropic compressibilities, $K_{S,m}^E$ and deviations in speed of sound, u^D. The apparent and partial molar properties and their deviations at infinite dilution were also calculated. Viscosity data were used to compute deviations in viscosity, $\Delta\eta$ and excess Gibbs energy of activation of viscous flow, ΔG^{*E}. Furthermore, the change in free energy, ΔG, change in enthalpy, ΔH and change in entropy, ΔS of activation of viscous flow have also been calculated. A Redlich–Kister type equation was applied to fit the excess molar volumes and deviations in isentropic compressibility, speeds of sound and viscosities data. The FT-IR and ^{1}H NMR studies of all mixtures were also reported.

1. Introduction

Mixed solvents provide a wide range of desired properties, which are frequently used as media for many chemical, industrial and biological processes. The knowledge of the volumetric, acoustic and transport properties of non-aqueous binary liquid mixtures has significance in the field of molecular modeling and drug designing [1,2]. Attention on mixtures of alkoxyalkanols + alcohols is a consequence of their broad variety of applications. Solutions of alcohols (refrigerant) with absorbents as alkoxyalkanols have been anticipated as working fluids for absorption refrigerant machines in order to improve the cycle machine [3]. This type of systems are used as gasoline additives due to their octane-enhancing and pollution reducing properties [4,5]. Alkoxyalkanol + alcohol mixtures are industrially relevant because alcohols are basic components in the synthesis of oxaalkanes. Mixtures of short chain 1-alkanols with alkoxyalkanols are also interesting; they can be considered as simple models of the complex systems, widely used in biochemical and biomedical processes [6]. The principal mark of our work is to bring a contribution to the knowledge of certain thermodynamic properties in the binary mixtures containing alkoxyalkanols and alcohols. From a theoretical point of view, the study of alkoxyalkanol + alcohol mixtures is particularly important due to their complexity, related to the partial destruction of the H-bonds between alcohol molecules by the active alkoxyalkanol molecules, and to the new OH···O bonds created upon mixing [7]. The binary mixtures of (alkoxyalkanols + alcohols) have been studied extensively and systematically in recent years. Recently, Pal and Gaba [8–10] have studied volumetric, acoustic and transport properties of the binary mixtures of 1-tert-butoxy-2-propanol, +1-propanol, +1-butanol and +2-butanol at 298.15 K.

In an effort to make a comprehensive study, we measure the densities, ρ and speeds of sound, u for the binary liquid mixtures containing alkoxyalkanols i.e. 1-tert-butoxy-2-propanol with alcohols at temperatures of (293.15, 298.15, 303.15, 308.15 and 313.15) K and viscosities, η at temperatures of (298.15, 303.15 and 308.15) K over the entire composition range. From the data, thus obtained, various properties have been derived. The changes in derived properties with composition and temperature of the mixtures have been discussed in terms of molecular interactions. The effect of the number of carbon atom and position of the −OH group in these alcohols on molecular interactions in these mixtures has also been discussed. In addition to this, IR and NMR spectra of pure components and their equimolar mixture are recorded. The spectroscopic studies (FT-IR and ^{1}H NMR) reveal the existence of specific interactions by examining the change in position of −OH group and bandwidth and by determination of chemical shift δ.

2. Experimental

2.1. Materials

1-Tert-butoxy-2-propanol was obtained from Sigma Aldrich. All alcohols i.e. 1-propanol (Analytical reagent grade), 2-propanol (Extra

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pure grade), 1-butanol (HPLC and spectroscopic grade) and 2-butanol (Analytical reagent grade) were procured from S.D. Fine Chemicals, India. Molecular structure and molecular mass of 1-tert-butoxy-2-propanol and alcohols are given in Scheme 1. All the chemicals were fractionally distilled and dried over 0.4 nm molecular sieves. The provenance and mass fraction purities tested by gas chromatography were reported in Table 1. The mass percentage water content by Karl-Fischer analysis of the chemicals was found to be 0.02%. The purities of solvents were further ascertained by comparing their densities, viscosities and speeds of sound at 298.15 K temperature with values reported in the literature [9,11–18] as shown in Table 2.

Table 1
Specification of chemical samples.

Chemical name	Provenance	Mass fraction purity
1-Tert-butoxy-2-propanol	Sigma Aldrich, India	0.995
1-Propanol	S.D. Fine Chemicals, India	0.995
2-Propanol	S.D. Fine Chemicals, India	0.998
1-Butanol	S.D. Fine Chemicals, India	0.997
2-Butanol	S.D. Fine Chemicals, India	0.995

2.2. Methods

Each of the binary mixtures was prepared by weighing appropriate amounts of 1-tert-butoxy-2-propanol and each alcohol mentioned above on an A&D Company limited electronic balance (Japan, Model GR-202) electronic balance, with a precision of ± 0.01 mg, by syringing each component into airtight narrow mouthed stoppered bottles to minimize evaporation losses. The pure components were separately degassed shortly before sample preparation. The probable error in mole fraction was estimated to be less than $\pm 1 \times 10^{-4}$.

2.3. Density and speed of sound measurements

Densities, ρ and speeds of sound, u were measured by using a digital vibrating tube density and speed of sound analyzer (Anton Paar DSA 5000). The details of calibration of the instrument and the experimental procedure have been described elsewhere [19–22]. The speed of sound is measured using a propagation time technique. The sound speed cell consists of a circular cavity 8 mm in diameter and 5 mm deep. The sample is sandwiched between two piezoelectric ultrasound transducers. One transducer emits sound waves through the sample-filled cavity at a frequency of approximately 3 MHz; the second transducer receives those waves. Thus, the speed of sound is obtained by dividing the known distance between transmitter and receiver by the measured propagation time of the sound wave [23]. Uncertainty in density measurement is $\pm 2 \times 10^{-3}$ kg m^{-3} and for the speed of sound is ± 0.1 m s^{-1}. The reliability of experimental measurements of ρ and u was ascertained by comparing the experimental data of pure liquids with the corresponding literature values (Table 2).

2.4. Viscosity measurements

The kinematic viscosities ν $(=\eta/\rho)$ of pure liquids and liquid mixtures were measured at (298.15, 303.15 and 308.15) K and at atmospheric pressure using an Ubbelohde suspended level viscometer. The uncertainty in the viscosity measurements, based on our work on several pure liquids, was ± 0.06 mPa s. The details of the methods used to determine viscosity have been described in our earlier publications [19–21]. The reliability of experimental measurements of ρ, η and u was ascertained by comparing the experimental data of pure liquids with the corresponding literature values (Table 2).

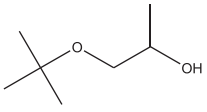
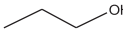
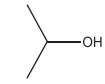
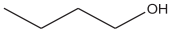
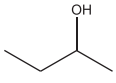
2.5. Spectral analysis

The Fourier transform infrared (FT-IR) spectra of pure components and their equimolar mixture were recorded using an ABB Horizon (MB 3000) spectrometer. The NMR chemical shifts of pure components and their molar equimolar mixture for ^{1}H were observed with a Bruker FT-NMR spectrometer operating at 300 MHz. Details of measuring procedure have been given in our earlier publication [20–22]. All the data analyses were performed in Microsoft Excel and Origin 6.1 software.

3. Results and discussion

The excess molar volumes, V^E_m, excess molar isentropic compressibilities $K^E_{S,m}$ and deviations in speed of sound u^D have been computed using

Scheme 1. Molecular structure and mass of chemical samples.

Sr. no.	Compound	Molecular structure	Molecular mass/(g·mol^{-1})
1.	1-Tert-butoxy-2-propanol	 $(CH_3)_3COCH_2CH(OH)CH_3$ $(CH_3)_3COCH_2CH(OH)CH_3$	132.20
2.	1-Propanol	 $CH_3(CH_2)_2OH$ $CH_3(CH_2)_2OH$	60.10
3.	2-Propanol	 $CH_3CH_2(OH)CH_3$ $CH_3CH_2(OH)CH_3$	60.10
4.	1-Butanol	 $CH_3(CH_2)_3OH$ $CH_3(CH_2)_3OH$	74.12
5.	2-Butanol	 $CH_3CH_2CH_2(OH)CH_3$ $CH_3CH_2CH_2(OH)CH_3$	74.12

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