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Densities, speed of sound, and IR studies of Ethyl lactate with 2-alkoxyethanols at different temperatures

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ABSTRACT

Densities and speeds of sound of the binary liquid mixtures of Ethyl lactate (EL) with 2-methoxyethanol (2-ME), 2-ethoxyethanol (2-EE) and 2-butoxyethanol (2-BE) have been measured over the entire composition range at temperatures of 303.15–318.15 K. From the experimental values excess molar volume (V_m^E), excess partial molar volume ($\bar{V}_{m,1}^E$, $\bar{V}_{m,2}^E$), excess partial molar volume at infinite dilution $(\upsilon_1^E)^\infty$, $(\upsilon_2^E)^\infty$ and excess isentropic compressibility (K_s^E) are computed. The variation with the temperature and concentration is discussed in terms of molecular interactions. The excess molar volume and excess isentropic compressibility parameters are fitted to Redlich–Kister polynomial equation to estimate the binary interaction parameters. Thermodynamic studies of the present binary systems reveal strong inter molecular interactions between the unlike molecules. The strength of intermolecular interaction between EL and 2-alkoxyethanol molecules is found to follow the order EL + 2-BE > EL + 2-EE > EL + 2-ME. The FT-IR analysis at various concentrations of these binary mixtures also suggest specific interaction between the unlike molecules and supported thermodynamic findings.

1. Introduction

Liquid mixtures are often used as channel for many chemical, industrial and biological processes because they provide a wide range of properties. Expertise of thermodynamic and acoustic properties of the liquid mixture is essential in understanding the nature and extent of the patterns of molecular aggregation that exist in binary liquid mixtures due to their sensitivities to variations in composition and the molecular structure of the pure components [1,2]. The experimental data of excess thermodynamic properties of liquid mixture provides knowledge about the type and magnitude of molecular interactions and can be used for the development of molecular models for describing the behaviour of solutions [3,4]. The thermo physical properties combined with spectroscopic studies give an extensive study of intermolecular interactions in the constituent binaries. Thermodynamic properties of binary liquid mixtures formed by two or more components associated through hydrogen bonds are interesting and important from both theoretical and process design aspects [5]. Spectroscopic technique like FT-IR is used to find out the existence of intra and inter molecular hydrogen bonds. It is a successful method to investigate the molecular structure of association effects among molecules.

Alkyl lactates (AL) are one of the fascinating classes of solvents due to unique physicochemical properties such as high boiling point, low surface tension and low vapour pressure. Ethyl lactate (EL) is the main member of the lactate esters family. EL is renewable, fully biodegradable, non-toxic, non-ozone depleting, and without any potential health risks [6]. It readily undergoes metabolic hydrolysis because of esterase enzymatic activity to ethyl alcohol and lactic acid. Ethyl lactate has the ability to dissolve a wide range of chemicals. It can be used to remove greases, silicone oils, and adhesives in cleaning a variety of metal surfaces for fabrication and coating applications. It is used as a cleaning solvent for the manufacturing of magnetic [7] and electronic devices [8]. Since the presence of Ethyl lactate exists in beer, wine, and soy products, it has been approved by the FDA for use in food industries for years. Moreover, Ethyl lactate has replaced solvents such as toluene, acetone xylene, N-methyl pyrrolidone and several harmful and halogenated chemicals. From a productive viewpoint, the

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Table 1
Materials description.

Component	Source	Purification method	Mass fraction purity	Purity analysis method
EL (racemic mixture)	Sigma–Aldrich	None	0.980	GC
ME	SD-fine	Fractional distillation	>0.995	GC
EE	SD-fine	Fractional distillation	>0.995	GC
BE	SD-Fine	Fractional distillation	>0.995	GC

replacement of traditional solvents by EL is clearly advisable considering that the recently developed technologies [9–11] allow its production from carbohydrate feed stocks at very low and competitive prices.

Alkoxyethanols viz. 2-methoxyethanol (2-ME), 2-ethoxyethanol (2-EE) and 2-butoxyethanol (2-BE) also known as cellosolves form another captivating class of compounds since they show rare characteristic of having ether, alcohol and hydrocarbon chain in the same molecule [12]. This give rise to the formation of intra and intermolecular hydrogen bonds which makes them self-associated. They can be used as valid model for the research of the hydration of polyether (PEO) which is important in many industrial, environmental and biological applications [13]. They are used as additives to gasoline due their octane enhancing and pollution reducing properties [14,15]. These solvents are used as cleansing liquids for removing exhaust air and gas streams from industrial production plants. The effective dipole moment of cellosolves is a useful measure to study the impact of polarity on bulk properties [16–18] and is found to be higher than that of the homo morphic 1-alkanol [19].

In continuation of our previous work [20–22] on phase equilibrium and excess thermodynamic properties, the present work aims at acoustic and volumetric properties of binary mixtures of Ethyl lactate with 2-alkoxyethanols in the temperature range 303.15–318.15 K at atmospheric pressure. A survey of literature shows that only a few combinations of EL liquid mixtures are studied and reported. Chen et al. [23] studied densities and viscosities of binary mixture of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate. Garcio et al. [24] investigated aqueous solutions of alkyl lactate at 298.15 K using thermophysical and spectroscopic properties. VLE studies and thermodynamic properties were carried out for binary mixtures of EL with acetates and alcohols by Resa et al. [25,26]. Lomba et al. [27] compared thermophysical behaviour of methyl, ethyl and butyl lactate in terms of intermolecular interaction. To the best of our knowledge there has been no literature report on acoustic and volumetric properties of binary mixtures of EL with 2-alkoxyethanols. This fact prompted the authors to carry out the research work on the above systems. To investigate the nature of the interactions various thermodynamic parameters, like excess molar volume, excess partial molar volume, excess partial molar volumes at infinite dilution and excess isentropic compressibility are calculated by using the density and speed of sound data. The effect of temperature and composition on molecular interaction is assessed and the influence of hydrogen bond on excess properties of the binaries is studied by using FT-IR. The excess molar volume and excess isentropic compressibility of all binary mixtures are correlated with the Redlich–Kister polynomial equation [28].

2. Experimental

2.1. Materials

Ethyl lactate (EL) is supplied by Sigma–Aldrich. The mass fraction purity is 0.980. The purity of the racemic mixture is checked using gas chromatography. It is used without further purification because the impurities are at a low concentration so that physical properties are almost unaltered within the quoted uncertainty limit [29]. The alkoxyethanols are supplied by SD Fine Chemicals Ltd. which is of analytical grade. The mass fraction purity for the chemicals is >0.995. These liquids are dried over 4°. A molecular sieves to reduce water content and partially degassed prior to their experimental use. 2-Alkoxyethanols are further purified by using the method described in the literature [30]. The chemicals used in the experiment are listed in Table 1. For comparing the purity of the liquids their densities and velocities are checked with those reported in the literature. The values are found in good agreement with literature values [31–37] provided in Table 2.

2.2. Apparatus and procedure

By mixing known weight of pure liquids the binary mixtures are prepared in air tight stoppered bottles as a precaution to minimize evaporation losses. The measurements of weight are done using an electronic balance (Shimadzu Analytical Balance, Japan. Model: AUW-120D) with accuracy ±1.10^{-4}. Rudolph Research Analytical DDM 2911, with automatic viscosity correction, is used for density measurements. The temperature in the cell is automatically controlled within ±0.02 K with a solid state thermostat (Peltier-type) and before each series of measurements it is calibrated at the atmospheric pressure. The calibration is done by using ambient air and bi-distilled ultrapure water (pH-5.3, conductivity-1.2 microseimens/cm). Moisture adsorbent is incorporated in the instrument. Each experimental density value is the average of at least three measurements at temperatures from 303.15 to 318.15 K. The densities of the samples are observed with reproducibility within 0.01% and an average value is reported. The samples for the measurement are immediately used after preparation. The speeds of sound in pure liquids and in their binary mixtures are measured using single-crystal variable-path ultrasonic interferometer (Mittal Enterprises, New Delhi, Model, M-81) operating at 2 MHz, calibrated with bi distilled water, methanol and benzene at 298.15 K. For all the measurements, temperatures were controlled by circulating water through an ultra thermostat (supplied by Mittal enterprises) keeping fluctuations within ±0.02 K. In all the measurements pressure is maintained at 0.1 MPa. Infrared spectra of all the three binary mixtures over the entire composition range were recorded at room temperature using Bruker FT-IR spectrophotometer (Germany), alpha-T with universal module, operated by opus software, in the frequency range 4000–400 cm^{-1}.

3. Theory

The measured values of density (ρ) and speed of sound (u) are used to determine acoustic and thermodynamic parameters like molar volume, partial molar volume and isentropic compressibility

Excess molar volume

$$V_m^E = [(x_1M_1 + x_2M_2)/\rho - x_1M_1/\rho_1 - x_2M_2/\rho_2] \quad (1)$$

Where x_1, x_2, M_1, M_2, ρ_1, and ρ_2 are mole fractions, molar masses, densities of pure components 1 and 2 respectively and ρ is the density of the liquid mixture.

Excess molar volume studies are further upholded by studying partial molar volumes. The partial molar volumes of components