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Density, sound velocity, viscosity, and refractive index of new morpholinium ionic liquids with amino acid-based anions: Effect of temperature, alkyl chain length, and anion

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ABSTRACT

In this work, room temperature synthesis of twenty new ionic liquids (ILs) based on the *N*-alkyl-*N*-methylmorpholinium ([$Mor_{1,R}$], R = 2, 3, 4, 6, 8) cation and *N*-acetyl-L-amino acid anions (L-alaninate, L-valinate, L-leucinate, L-isoleucinate) was described. The synthesized ILs were characterized by various spectroscopic techniques and high-resolution mass spectrometry. Furthermore, density (ρ), sound velocity (v), viscosity (η) and refractive index (n_D) have been measured within the temperature range of T = (298.15 to 318.15) K and at 0.1 MPa pressure. The density, sound velocity and viscosity values were fitted to linear and Vogel–Tammann–Fulcher (VTF) equation. Moreover, on the basis of the refractive index values, molar refraction (R_m) and free volume (V_f) were calculated using the Lorentz–Lorenz equation. The thermodynamic properties such as thermal expansion coefficient (α) and isentropic compressibility (κ_S) were calculated using the experimental values of density and sound velocity. Finally, the obtained data were evaluated in order to determine the effect of such parameters as temperature, the nature of the anion and the length of the cation alkyl chain.

1. Introduction

Ionic liquids (ILs) are organic salts consisting entirely of ions that are normally liquids at or close to room temperature (by definition below 100 °C). ILs have attracted a great deal of attention throughout the last twenty years due to their unique physicochemical features, including negligibly low vapour pressure, broad temperature range in the liquid state, high thermal stability, high viscosity and density, and affinity to organic or inorganic compounds [1]. The popularity of these molten salts as alternatives to traditional harmful organic solvents is not only due to their promising properties, but also due to their tunability. In contrast to molecular liquids, ILs should be considered complex systems, wherein independent properties of the ions as well as their interactions play essential roles. Most of the aformentioned features of ILs are related to the presence of strong Coulombic forces. Additional attractive or repulsive forces that affect anion–cation systems include hydrogen bonds, π-π interactions, ion–dipole, ion–induced dipole, and permanent dipole interactions, as well as dispersion forces. The excellent properties obtainable by modification of ILs enable their application in many different fields of science and technology [2–4]. In the last decade, there has been a new direction in research on ILs emphasizing the preparation of "object-oriented" or "task-specific" ILs [5].This involves design of the IL structure with regard to the purpose or field of application. The synthesis of dedicated ILs is a great challenge, and requires studies of the physicochemical properties of the IL family for a better understanding of the relationship between their structure and properties. The immense number of possible ILs demands the development of predictive models to identify an appropriate IL for a given application [6].Therefore, a relatively broad, systematic, and sufficiently accurate dataset of properties is required for known, as well as new, ILs [7–10]. Although a big amount of data on the physicochemical properties of ILs has been already published, systematic studies are still necessary, and this topic should be further explored.

The effective design of industrial and laboratory processes involving ILs requires a thorough understanding of their physicochemical properties, such as density, viscosity, and refractive index [11].The density and viscosity of ILs often provide a reference point for the determination of other parameters that play key roles in defined chemical process, such as rates of liquid-liquid phase separation and mass transfer, or power requirements of mixing and pumping [12]. For example, the density of an IL must be known in order to solve the material or energy balance equations of an industrial chemical process [13]. On the other hand, refractive index of ILs is more linked to specific chemical properties like polarity and relative hydrogen bond donating and accepting ability, which are used to determine solubility, partition constants and reaction

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