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Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure

S. Govardhana Rao [a,*], T. Madhu Mohan [b], T. Vijaya Krishna [b], B. Subba Rao [c]

[a] Department of Physics, St. Mary's Group of Institutions Guntur, Guntur, Andhra Pradesh, India
[b] Department of Physics, Vasireddy Venkatadri Institute of Technology, Nambur, Andhra Pradesh, India
[c] Department of Physics, VSR & NVR College, Tenali, Andhra Pradesh, India

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ABSTRACT

Density (ρ), refractive index (n_D) and speed of sound (u) values are measured for the binary mixture of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone over the entire range of mole fraction at temperatures from (298.15 to 323.15) K under atmospheric pressure. Using the basic experimental data, molar volume (V_m), isentropic compressibility (k_s), intermolecular free length (L_f), molar refraction (R_m), excess molar volume (V_m^E), excess isentropic compressibility (κ_s^E) and excess intermolecular free length (L_f^E) values are calculated. The calculated properties are discussed in terms of molecular interactions between the present investigated system. The excess values are fitted to Redlich–Kister polynomial equation to estimate the binary coefficients and standard deviation between the experimental and calculated values. Further, the molecular interactions in the binary mixture system are analysed using the experimental FT-IR spectrum recorded at room temperature.

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1. Introduction

Ionic liquids (ILs) have recently emerged as "green" and environment friendly solvents for their use in the industrial manufacture of chemicals. In the past decade, ionic liquids have been increasingly used for diverse applications such as organic synthesis, catalysis, electrochemical devices and solvent extraction of a variety of compounds [1,2]. The interest in ILs was initiated because of their advantageous physico-chemical properties such as negligible vapour pressure, high thermal and electrochemical stability, high solvating power, *etc.* Further, ILs are good solvents for a whole range of organic and inorganic materials and some of them are immiscible with organic solvents and therefore they provide a polar alternative with non-aqueous nature for two-phase systems.

Ionic liquids are composed of cations and anions having low melting point (<100 °C). While the cations may be organic or inorganic, the anions are inorganic. The choice of the cation and the anion constituting an IL has a profound effect on the physical properties such as density, refractive index, speed of sound, dielectric permittivity, conductivity, polarity, *etc.* ILs offer a great flexibility in their properties since the possible combinations of cations and anions are quite high. The physico-chemical properties of the ILs can be finely tuned by changing the cation or the anion. Thus, novel solvents can be formed and can be used for a specific application which cannot be done with the conventional organic solvents. The information regarding the thermophysical properties of pure ILs as well as their mixtures with other compounds is essential for the designing and development of equipment for commercial applications such as batteries, photoelectric cells, solar cells and so forth [3–7].

The present work is aimed at studying the molecular interactions in the binary mixture of the IL–1-butyl-3-methylimidazolium tetrafluoroborate ([Bmim][BF_4]) with 2-pyrrolidone (2-Py). Imidazolium based ILs can be used for extractive desulfurization of liquid fuels, mainly with regard to those S-compounds that are very complicated to eliminate by common hydrodesulfurization (HDS) process. [Bmim][BF_4] is most efficient in the removal of dibenzothiophene (DBT) containing liquid fuels [3]. The structure of 2-pyrrolidone is of great interest as it is related to many structural problems in molecular biology. The self-association of 2-pyrrolidone serves as a model for hydrogen bonding in nucleic acid amides. The compound 2-pyrrolidone is used as a solvent for surface treatment for textiles, metal coated plastics, polymers, and paint removing. It is also used as

* Corresponding author. Tel.: +91 9885193953; fax: +91 0863 2293699.
E-mail address: sgovardhan104@gmail.com (S. Govardhana Rao).

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an intermediate in the production of vinylpyrrolidone and drug piracetam.

2. Experimental

2.1. Materials

The compound 1-butyl-3-methylimidazolium tetrafluoroborate ([Bmim][BF_4]) is procured from Io-Li-Tec, Germany. Before using, [Bmim][BF_4] is dried under vacuum [2] for more than 12 h at $T = 343.15$ K and the water content in [Bmim][BF_4] is found to be $320 \cdot 10^{-6}$. The 2-pyrrolidone (2-Py) is procured from Sigma Aldrich, USA and is purified by fractional distillation method under reduced pressure. The water content is measured using Analab (Micro Aqua Cal 100) Karl Fischer Titrator and Karl Fischer reagent from Merck, by conductometric titration with dual platinum electrode. It can detect water content from less than $10 \cdot 10^{-6}$ to 100% [8]. The provenance, CAS number, water content and mass fraction purity values of the compounds are given in table 1. The purity of the chemicals is ascertained by comparing the experimental values of density, refractive index and speed of sound at temperatures $T = (298.15$ to $323.15)$ K with the NIST ThermoLit data (table 2) [2,4–7,9–29].

2.2. Apparatus and procedure

The binary mixture is prepared by weighing appropriate amounts of pure liquids on a digital electronic balance (Mettler Toledo AB 135, Switzerland) with an uncertainty of $\pm 1 \cdot 10^{-8}$ kg, by syringing each component into airtight stopper glass vials with [Bmim][BF_4] and 2-Py. The vials are closed with screw caps ensuring a secure seal and to prevent humidity. The mixture of the various compositions are freshly prepared and taken from the vial with the syringe and then are put into an apparatus immediately to prevent the mixture from atmospheric moisture. The uncertainty in the mole fraction of all mixtures is estimated to be less than ±0.005. Density, refractive index and speed of sound are measured at the same time using the same samples to reduce the experimental error.

TABLE 1
Provenance, CAS number, water content and mass fraction purity of the chemical used in the study.

Chemical	Provenance	CAS number	Water content	Initial mass fraction purity (by supplier)	Purification method	Final mass fraction purity	Analysis method
1-Butyl-3-methylimidazolium tetrafluoroborate	Io-Li-Tec, Germany	174501-65-6	$320 \cdot 10^{-6}$	0.99	Vacuum Treatment	0.99	NA
2-Pyrrolidone	Sigma Aldrich, USA	616-45-5	$300 \cdot 10^{-6}$	0.990	Distillation	0.994	(Gas + liquid) chromatography

TABLE 2
Comparison of experimental density (ρ), refractive index (n_D) and speed of sound (u) of pure compounds with literature values at temperatures from $T = (298.15$ to $323.15)$ K at pressure $P = 0.1$ MPa.

Compound	T/K	ρ/kg · m^{-3}		n_D		u/m · s^{-1}	
		Experimental	Literature	Experimental	Literature	Experimental	Literature
1-Butyl-3-methylimidazolium tetrafluoroborate	298.15	1198.78 [4]	1200.57 [5] 1200.60 [2] 1201.07 [6] 1194.60 [7]	1.42058 [4]	1.4197 [9] 1.4227 [10]	1565.09 [4]	1566 [6] 1565.1 [9] 1576.05 [11]
	303.15	1195.18 [4]	1196.98 [5] 1197.7 [2] 1190.44 [7] 1198.09 [12]	1.41913 [4]	1.4181 [9] 1.4214 [10]	1553.15 [4]	1552.6 [9] 1555.47 [11] 1544.88 [13]
	308.15	1191.60 [4]	1194.2 [14] 1194.8 [2]	1.41764 [4]	1.4166 [9] 1.4200 [10]	1541.35 [4]	1540.3 [9] 1543.92 [11]
	313.15	1188.04 [4]	1189.86 [5] 1190.99 [12] 1191.5 [2]	1.41621 [4]	1.4155 [9] 1.4192 [10]	1529.69 [4]	1528.3 [9] 1532.52 [11] 1525.22 [13]
	318.15	1184.50 [4]	1187.4 [14] 1188.4 [2]	1.41472 [4]	1.4142 [9] 1.4188 [10]	1518.19 [4]	1516.5 [9] 1521.19 [11]
	323.15	1180.98 [4]	1182.81 [5] 1183.95 [12]	1.41330 [4]	1.4132 [9] 1.4172 [10]	1506.80 [4]	1505.1 [9] 1503.36 [13]
2-Pyrrolidone	298.15	1107.16	1108.0 [15] 1107.01 [16] 1107.12 [17] 1106.97 [18]	1.48591	1.4853 [19]	1634.38	1633.2 [20] 1633.95 [18]
	303.15	1103.07	1103.4 [15] 1103.0 [21]	1.48403	1.4839 [22]	1617.97	1617.64 [21] 1615.79 [23]
	308.15	1098.99	1099.15 [16] 1099.13 [17] 1097.14 [24]	1.48218	1.4822 [25]	1601.62	1603.0 [26] 1599.97 [24]
	313.15	1094.90	1095.0 [15] 1095.18 [17] 1095.27 [27]	1.48033	1.4805 [25] 1.48467 [28]	1585.44	
	318.15	1090.82	1091.05 [15] 1091.01 [17]	1.47841	1.4790 [25]	1570.39	1563.2 [20]
	323.15	1086.75	1086.9 [15] 1087.1 [29]	1.47649	1.4769 [22] 1.4775 [25]	1553.48	

Standard uncertainties u are $u(T) = \pm 0.01$ K, $u(\rho) = \pm 0.5$ kg · m^{-3}, $u(n_D) = \pm 0.0004$, $u(u) = \pm 0.5$ m · s^{-1}, $u(P) = \pm 0.008$ MPa.

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