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Cibulka correlation for ternary excess/deviation properties of {[C_2mim][$EtSO_4$] (x_1) + acetic or propionic acid (x_2) + acetonitrile (x_3)} systems at different temperatures

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ABSTRACT

In this perspective, the main intention is to reveal the possible intra and inter molecular interactions between ternary ionic liquid systems. The excess molar volume (V^E_{123}), isentropic compressibility (k_s) and deviation in isentropic compressibility (Δk_{s123}) were determined for two ternary liquid mixtures of {[C_2mim][$EtSO_4$] (x_1) + acetic or propionic acid (x_2) + acetonitrile (x_3)} at different temperatures (293.15, 298.15, 303.15, 308.15 and 313.15) K and at $p = 1 \times 10^5$ Pa with the aid of the experimental density (ρ) and speed of sound (u) measurements. The calculated ternary excess volume and deviation in isentropic compressibility results were correlated by using the Cibulka equation with the aid of Redlich–Kister parameters obtained from literature corresponding binary systems. Furthermore, the measured thermodynamic properties are discussed in terms of molecular interactions between component molecules in liquid mixtures.

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1. Introduction

From past decades, ionic liquids (ILs) are considered as the new class of eco-friendly solvents for the replacement of commonly used volatile organic liquids. ILs commonly consist of organic cations and inorganic or organic anions with melting point below the boiling point of water [1–4]. The ILs are used in many disciplines of science and industries due to their beneficial properties *viz.* chemical stability, high ionic mobility, non-flammability, thermal stability, low vapour pressure, good solubility in various solvents and high potential for recycling [5–10]. For example, the imidazolium based ILs have been used in chemical synthesis, electrochemical technology, extraction process, bio-catalysis and separation science [11–15]. Also these ILs have been used extensively in related protein–DNA, liquid crystals, nano-materials, chromatography, mass spectrometry and materials for embalming [16–18]. Other system components, *i.e.* acetic acid and propionic acid are solvents, which have extensive applications in various industries, are especially used in chemical industries as an intermediate for the production of different chemicals and in polymer, plastic and cosmetics industries [19]. Similarly, acetonitrile has been employed in refineries purification, storage batteries, cyclic voltammetry, synthesis of DNA oligonucleotides and drug products [20].

The thermophysical properties of ILs are useful to help understand the fundamental knowledge of significant aspects of solution chemistry as they result from the molecular interactions [21–25]. Furthermore, knowledge of these thermophysical properties of liquid mixtures are necessary in the process design in many industrial applications such as surface facilities, pipeline systems, heat transfer, mass transfer, fluid flow and biomedical research [26–32]. Moreover, the thermodynamic properties of liquid mixtures play an important role to understand the specific interactions, geometrical effects, molecular arrangements and molecular modelling between component molecules [33–37].

In the present investigation, we report density (ρ), excess molar volume (V^E_{123}), speed of sound (u), isentropic compressibility (k_s) and deviation in isentropic compressibility (Δk_{s123}) for two ternary liquid mixtures containing {[C_2mim][$EtSO_4$] (x_1) + acetic or propionic acid (x_2) + acetonitrile (x_3)} at temperatures ranging from 293.15 to 313.15 K in steps of 5 K and at $p = 1 \times 10^5$ Pa. Consequently, in order to investigate systematically the nature of interactions between the imidazolium-based ILs and different functional groups of organic solvents, knowledge of thermodynam-

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ics of solution is required. Furthermore, we discuss molecular interactions between component molecules and examine the influence of temperature on the thermophysical and thermodynamic properties.

2. Experimental

2.1. Materials

All the chemical substances were purchased from Sigma-Aldrich Chem. The mass fraction purity of all chemicals used in this study was ⩾0.99. Prior to making the experimental measurements, all the chemicals were degassed by ultrasound for over 3 h, kept out of the light over Fluka 0.3 nm molecular sieves for several days. The water content of liquids used in this work was measured by Metrohm 702 SM Titrino Metter. The source, CAS number, mass fraction water content and purity of chemicals are listed in Table 1. The purities of the ionic liquid and other solvents used in this work were verified by comparing the densities and sound velocities measured in our previous publications [38,39] at various temperatures. Furthermore, the purities of ionic liquids and other solvents were confirmed by GC analysis.

Table 1
Provenance and purity of the materials used.

Component	Source	CAS number	Purification method	Water content mass percent	Mass fraction purity	
					Initial	GC analysis (final)
$[C_2mim][EtSO_4]$	Aldrich	342573-75-5	Degassed by ultrasound, kept out of the light over Fluka 0.3 nm molecular sieves for several days; water content were checked before and after by Karl-Fischer titration	0.05	⩾0.990	>0.990
Acetonitrile	Aldrich	75-05-8	–	0.10	⩾0.990	>0.990
Acetic acid	Aldrich	64-19-7	–	0.03	⩾0.990	>0.990
Propionic acid	Aldrich	79-09-4	–	0.02	⩾0.995	>0.995

The mass percent water content was determined using a Metrohm 702 SM Titrino Metter before the experiments.

Table 2
Density (ρ), speed of sound (u), excess volume (V^E_{123}), isentropic compressibility (k_s) and deviation in isentropic compressibility (Δk_{s123}) for {$[C_2mim][EtSO_4]$ (x_1) + acetic or propionic acid (x_2) + acetonitrile (x_3)} at (293.15–313.15) K and at $p = 1 \times 10^5$ Pa.

x_1	x_2	ρ/g cm^{-3}	V^E_{123}/cm^3 mol^{-1}	u/m s^{-1}	k_s/(10^8 Pa)$^{-1}$	(Δk_{s123}) (10^8 Pa)$^{-1}$
{$[C_2mim][EtSO_4]$ (x_1) + acetic acid (x_2) + acetonitrile (x_3)}						
T = 293.15 K						
0.0680	0.5284	1.01469	−0.933	1336.7	55	−15.2
0.1009	0.2975	0.99452	−1.052	1382.8	53	−17.2
0.1126	0.2205	0.98910	−1.104	1395.8	52	−17.6
0.1290	0.1085	0.98111	−1.197	1411.4	51	−18.0
0.1672	0.3906	1.06174	−1.010	1432.3	46	−20.3
0.2126	0.2277	1.06194	−1.089	1470.8	44	−21.2
0.2325	0.1539	1.06205	−1.161	1484.5	43	−21.4
0.1038	0.7936	1.09557	−0.828	1355.8	50	−17.9
0.2309	0.5332	1.11957	−0.889	1479.1	41	−21.8
0.3114	0.3618	1.13002	−0.961	1527.5	38	−21.5
0.3560	0.2933	1.13814	−0.974	1548.0	37	−21.0
0.3980	0.1998	1.14191	−1.041	1566.8	36	−20.3
0.4538	0.0964	1.14820	−1.065	1588.9	34	−19.3
0.3450	0.5414	1.16434	−0.716	1541.4	36	−21.0
0.4835	0.3567	1.18325	−0.703	1594.3	33	−18.0
0.5604	0.2535	1.18992	−0.535	1619.7	32	−16.0
0.6545	0.1295	1.19819	−0.471	1643.1	31	−13.2
0.7078	0.0525	1.20237	−0.524	1652.1	30	−11.4
0.8825	0.0606	1.22942	−0.101	1678.5	29	−4.6
0.6002	0.3617	1.20906	−0.475	1624.7	31	−14.4
0.4887	0.4803	1.19712	−0.586	1594.2	33	−17.7
0.8075	0.1402	1.22505	−0.223	1666.6	29	−7.3
0.7287	0.2257	1.21984	−0.329	1652.7	30	−10.1
0.3492	0.6287	1.17464	−0.491	1532.9	36	−20.3
0.2108	0.7759	1.14861	−0.836	1456.7	41	−21.5
T = 298.15 K						
0.0680	0.5284	1.00984	−0.973	1320.4	57	−16.2
0.1009	0.2975	0.98985	−1.100	1366.3	54	−18.2
0.1126	0.2205	0.98449	−1.155	1379.3	53	−18.7
0.1290	0.1085	0.97653	−1.249	1394.7	53	−19.1
0.1672	0.3906	1.05743	−1.068	1416.2	47	−21.5
0.2126	0.2277	1.05768	−1.146	1455.5	45	−22.4
0.2325	0.1539	1.05783	−1.219	1469.3	44	−22.6
0.1038	0.7936	1.09092	−0.868	1340.5	51	−19.0
0.2309	0.5332	1.11539	−0.939	1464.6	42	−23.0
0.3114	0.3618	1.12601	−1.013	1513.4	39	−22.7
0.3560	0.2933	1.13420	−1.026	1533.8	37	−22.1
0.3980	0.1998	1.13802	−1.092	1552.8	36	−21.4
0.4538	0.0964	1.14439	−1.117	1575.4	35	−20.3
0.3450	0.5414	1.16047	−0.766	1527.7	37	−22.1
0.4835	0.3567	1.17949	−0.743	1581.0	34	−19.0

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