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(p,ρ,T) Properties of 1-octyl-3-methylimidazolium tetrafluoroborate

JAVID T. SAFAROV[1,2]*, AYGUL T. NAMAZOVA[2], ASTAN N. SHAHVERDIYEV[2] and EGON P. HASSEL[1]

[1]Institute of Technical Thermodynamics, University of Rostock, Germany and [2]Department of Heat Energy, Azerbaijan Technical University, Baku, Azerbaijan

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Abstract: (p,ρ,T) data of 1-octyl-3-methylimidazolium tetrafluoroborate [OMIM][BF_4] over a wide range of temperatures, from 278.15 to 413.15 K, and pressures, p, up to 140 MPa are reported with an estimated ±0.01–0.08 % experimental relative average percent deviation (*APD*) in the density. The measurements were performed using an Anton Paar DMA HPM vibration tube densimeter. (p,ρ,T) Data for [OMIM][BF_4] was fitted and the parameters of the applied equation were determined as a function of pressure and temperature. After a thorough analysis of literature values and validity of the used equation of state, various thermophysical properties, such as isothermal compressibility, isobaric thermal expansibility, differences in isobaric and isochoric heat capacities, thermal pressure coefficient, internal pressure, heat capacities at constant pressure and volume, speed of sound and isentropic exponent at temperatures in the range 278.15–413.15 K and pressures p up to 140 MPa were calculated.

Keywords: ionic liquid; density; equation of state; thermal properties; caloric properties; speed of sound.

INTRODUCTION

Ionic liquids (ILs) have great importance due to their excellent thermophysical and chemical properties, such as negligible vapour pressure, large liquidus range, high ionic conductivity, and non flammability. These excellent properties of ILs make them very useful substances in chemical and mechanical engineering industries. They have large number of applications in catalytic biomass transformation, solvation technology, electronics, Li-ion batteries, the polymer industry, separation technology, liquid–liquid extraction *etc.*[1,2] Thermophysical, electro- and physicochemical properties, *etc.* are very important for the analysis

* Corresponding author. E-mail: javid.safarov@uni-rostock.de
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and application of ILs. The most fundamental properties of ILs are (p,ρ,T) data, which were measured and presented in this paper, as well viscosity, heat capacity, speed of sound,[3] *etc.*, from which more parameters could easily be derived. This work is a continuation of ongoing investigations in the field of thermophysical properties of liquids at high pressures over a wide range of temperatures.[4–6] The (p,ρ,T) properties of 1-octyl-3-methylimidazolium tetrafluoroborate ([OMIM][BF_4]) over a wide temperature interval from 278.15 to 413.15 K and pressures p up to 140 MPa, using the high quality vibration tube densimeter method, were studied for the first time. The isothermal compressibility $\kappa_T(p,T)$, isobaric thermal expansibility $\alpha_p(p,T)$, thermal pressure coefficient $\gamma(p,T)$, internal pressure $p_{\mathrm{int}}(p,T)$, specific heat capacities $c_p(p,T)$ and $c_v(p,T)$, speed of sound $u(p,T)$, isentropic exponent $\kappa_s(p,T)$ were calculated using an equation of state at these high pressures and over the wide range of temperature, in which the density of [OMIM][BF_4] was studied. For such investigations, high quality density values at high pressures and over a wide range of temperature and also the heat capacity of [OMIM][BF_4] at ambient pressure and over a wide range of temperatures are necessary.[3]

The measured density of [OMIM][BF_4] at high pressures and over a wide range of temperatures was thoroughly compared with available literature values[7–14] in order to confirm their quality; a summary is presented in Table S-I of the Supplementary material.

The information about the density $\rho(p_0,T)$, viscosity $\eta(p_0,T)$, heat capacity $c_p(p_0,T)$, speed of sound $u(p_0,T)$ measurements and literature analysis of [OMIM][BF_4] at ambient pressure were presented in a previous publication.[3] The previous high pressure literature $\rho(p,T)$ measurements covered pressures up to 10, 20, 60, 207 or 224 MPa in various studies. However, the temperature ranges of the measurements within these papers were not large (Table S-I of the Supplementary material to this paper). Gu and Brennecke,[7] in 2002, studied density $\rho(p,T)$ at 298 and 323 K and pressures to 206.94 MPa using an ultrahigh-pressure density apparatus. These were the first reported high pressure density values. Harris *et al.*,[8] in 2006, investigated the densities at pressures up to 224.2 MPa. Both works covered small temperature intervals. Gardas *et al.*,[9] in 2007, investigated experimental high pressure densities $\rho(p,T)$ over a wide range of temperatures using an Anton Paar DMA 60 digital vibrating-tube densimeter, with a DMA 512P measuring cell for high pressures. The derived thermodynamic properties, such as isothermal compressibility, isobaric thermal expansibility, thermal pressure coefficient, and pressure dependence of heat capacity were defined. Sanmamed *et al.*,[10] in 2010, presented densities at high temperatures and pressures using a DMA 512P vibrating tube densimeter. Tomida *et al.*,[11] in 2012, investigated the density $\rho(p,T)$ of [OMIM][BF_4] from 293.15 to 353.15 K and pressures from 0.1 to 20.0 MPa using a DMA 512P vibrating-tube densimeter.

These measurements did not cover wide ranges of temperatures and pressures simultaneously. Hosseini *et al*.,[12] in 2013, employed a perturbed hard-sphere chain equation of state (PHSC EOS) for modelling the density of [OMIM][BF_4]. The equation was employed over a wide range of temperatures and pressures from 313 to 452 K and from 0.1 to 10 MPa with 77 literature data points for [OMIM][BF_4]. Roshan and Ghader,[13] in 2013, presented two models for the calculation of the density of [OMIM][BF_4] at pressures from 1 to 10 MPa and in the temperature range 293.15 to 393.15 K. The first method was based on Taylor's series the volume expansion of IL and the second model was in the form of the Padé approximation of volume as a function of pressure. The number of given data points for [OMIM][BF_4] was 66, and an *APD* of 0.104 % for the Taylor and 0.199 % for the Padé method were indicated. Ribeiro *et al*.,[14] in 2014, measured the glass transition pressure of [OMIM][BF_4] at room temperature.

The isobaric heat capacities, $c_p(p,T)$, of [OMIM][BF_4] at high pressures had been presented only by Sanmamed *et al.*[10] at pressures up to 60 MPa.

Only two papers[8,11] included high pressure viscosity $\eta(p,T)$ values. Harris *et al*.,[8] in 2006, performed measurements of viscosity $\eta(p,T)$ between 273.15 and 353.15 K and pressures from 0.1 to 224 MPa using a falling-body viscometer. Modified Litovitz and Vogel–Fulcher–Tammann equations were used to present the temperature and pressure dependences. Tomida *et al*.,[11] in 2012, published experimental viscosity $\eta(p,T)$ values from 293.15 to 353.15 K and pressures from 0.1 to 20.0 MPa using a rolling-ball viscometer. The uncertainty of the reported viscosity values was estimated to be 1.6 %. The experimental viscosity data at high pressures were fitted to the Tait equation.

Navia *et al*.,[15] in 2010, measured the isobaric thermal expansivity $\alpha_p(p,T)$ from 278.15 to 348.15 K and pressures from 5 to 50 MPa using a Micro DSCII microcalorimeter from Setaram.

Analysis of literature density at high pressures and over a wide range of temperature[7–14] (Table S-I) shows the necessity of careful experimental (p,ρ,T) measurements of this IL and analysis of thermophysical properties over a wide range of temperatures and pressures, including temperatures below room temperature and at high pressures for the following reasons:

– There are no density values for pressures higher than p = 60 MPa and T = 353.15 K;

– There are no density values above T = 393.15 K;

– There is only one report[9] of heat capacity $c_p(p,T)$ data at high pressures;

There are no other values of thermophysical properties over a wide range of temperature and pressures except one.[15]

Therefore, it was decided to investigate the thermophysical properties of [OMIM][BF_4] over a wide range of temperatures 278.15–413.15 K and pressures from 0.1 to 140 MPa in combination with a thorough literature analysis.

EXPERIMENTAL

Pure [OMIM][BF_4] was purchased from Sigma–Aldrich, Germany (CAS No. 244193--52-0). The sample was degassed under vacuum and at high temperatures up to T = 423.15 K before the experiments (mass purity >99 %). The water content of [OMIM][BF_4] was determined using a Karl Fischer titration and found to be less than 40 ppm.

The (p,ρ,T) measurements are carried out using a new modernized high pressure–high temperature Anton Paar DMA HPM vibration tube densimeter.[16,17] The temperature in the measurement cell, where the U-tube is located, was controlled using a thermostat (F32-ME Julabo, Germany) with a ΔT = ±10 mK uncertainty of the temperature and was measured using a (ITS-90) Pt100 thermometer (type 2141) with a ΔT = ±15 mK experimental uncertainty in the measurement. The pressure was measured by pressure transmitters P-10 and HP-1 (WIKA Alexander Wiegand GmbH., Germany) with an *APD* of 0.1 and 0.5 %, respectively, of the measured maximum value. The sample in the oscillating tube is part of a complex system. The force of inertia shear forces occurs on the wall, influencing the resonant frequency of the oscillator. The mPDS2000V3 control unit measures the vibration period with an accuracy of $\Delta\tau$ = ±0.001 µs. According to the specifications of Anton−Paar and the results of the calibration procedures, the observed repeatability of the density measurements at temperatures from 273.15 to 413.15 K and pressures up to p = 140 MPa is within $\Delta\rho$ ±0.1–0.3 kg m^{-3} or an *APD* of 0.01–0.03 %. However, if samples of higher viscosities are measured, it could be noticed that the displayed density was too high. Up to a certain level, this error is a function of viscosity.[18,19] This behaviour could be explained by considering a segment of the oscillator in motion. Investigating a "slice" of sample, it is found that both translational and rotational movements occur. The force required to keep the slice rotating is introduced by shear forces on the wall. As the viscosity increases, an increasing part will rotate until the whole slice rotates like a solid body. The momentum of inertia of the rotated section when added to the force of inertia of the movement of translation, simulates a higher mass with respect to volume, and so a higher density value. A correction can easily be performed if the form of the error curve and the sample viscosity are known.[19,21] In the present work the viscosity correction $(\rho_{HPM}-\rho)/\rho_{HPM}$ was included in the density measurements as follows:[21]

$$\frac{\rho_{HPM}-\rho}{\rho_{HPM}} = 10^{-4}(0.4482\sqrt{\eta}-0.1627) \tag{1}$$

For evaluation of Eq. (1), $(\rho_{HPM}-\rho)/\rho_{HPM}$ as a function of viscosity η, which must be known in the same temperature and pressure range where the densities are determined, is required. Unfortunately, there was no possibility to investigate the viscosity of this IL at high pressures, which are necessary for the viscosity correction of (p,ρ,T) data considering the high viscosity values for ionic liquids. Only the dynamic viscosity $\eta(p_0,T)$ of [OMIM][BF_4] at ambient pressures[3] and in the temperature range 278.15–373.15 K was measured. The present measured values together with literature values of the dynamic viscosity at ambient pressure[3] $\eta(p_0,T)$ and at high pressures[8,11] $\eta(p,T)$, and an extrapolation of them to 278.15–413.15 K range and p = 140 MPa, were used during the calculation of viscosity correction $(\rho_{HPM}-\rho)/$ $/\rho_{HPM}$. The described uncertainty of the viscosity measurements in the literature and the application of these results to the temperature and pressure intervals of the present work increased the possible uncertainty of the density measurements of the present work. From the other point of view, the effect of the right side of Eq. (1) is small and the uncertainty increase in the density correction is not very large. Thus, the uncertainty of the density measurements could be predicted to be between $\Delta\rho$ of ±0.1 to 0.8 kg·m^{-3} or an *APD* of 0.01–0.08 %.

Additional experimental data are given in Supplementary material to this paper.

RESULTS

The (p,ρ,T) data for [OMIM][BF_4] at 278.15–413.15 K and pressures up to p = 140 MPa are reported in Table S-II of the Supplementary material. The temperature and pressure steps in the experiments were approximately 5 to 20 K and 5 to 10 MPa. The measured densities as a function of pressure and temperature were fitted to Eq. (2):[22]

$$p(\rho,T) = A(T)\rho^2 + B(T)\rho^8 + C(T)\rho^{12} \tag{2}$$

where the coefficients $A(T)$, $B(T)$ and $C(T)$ are functions of temperature:

$$A(T) = \sum_{i=1}^{4} a_i T^i \tag{3}$$

$$B(T) = \sum_{i=0}^{3} b_i T^i \tag{4}$$

$$C(T) = \sum_{i=0}^{3} c_i T^i \tag{5}$$

The coefficients a_i, b_i and c_i of Eqs. (3)–(5) are given in Table S-III of the Supplementary material. Within these comparisons, the percent (PD) and APD between the literature values and the present experimental density values were calculated as:

$$PD = 100\left(\frac{\rho_{\text{exp}} - \rho_{\text{lit}}}{\rho_{\text{exp}}}\right) \tag{6}$$

$$APD = \frac{1}{n}\sum_{i=1}^{n}\left|100\left(\frac{\rho_{\text{exp}} - \rho_{\text{lit}}}{\rho_{\text{exp}}}\right)\right| \tag{7}$$

where ρ_{exp} is the experimental density measured in this work, ρ_{lit} is the density values reported in the literature; n is the number of compared points.

Eqs. (2)–(5) describe the experimental results of density of [OMIM][BF_4] within APD $\Delta\rho/\rho$ = 0.011 %.

The plot of pressure p of [OMIM][BF_4] *versus* density ρ is shown in Fig. 1. The plots of the deviations of the experimental density $\rho_{\text{exp.}}$ of [OMIM][BF_4] from the density calculated using Eqs. (2)–(5) $\rho_{\text{cal.}}$ *versus* pressure p in 278.15–413.14 K are shows in Fig. S-I (Supplementary material).

The values of the isothermal compressibility $\kappa_T(p,T)$, isobaric thermal expansibility $\alpha_p(p,T)$, difference in isobaric and isochoric heat capacities $(c_p–c_v)(p,T)$, thermal pressure coefficient $\gamma(p,T)$, internal pressure $p_{\text{int}}(p,T)$, isobaric heat capacity $c_p(p,T)$, isochoric heat capacity $c_v(p,T)$, speed of sound u / m·s^{-1} and isentropic exponent $\kappa_s(p,T)$ of [OMIM][BF_4] were calculated from Eqs. (S-1)–(S-12) of the Supplementary material, using fundamental equations of thermodynamics[4,23,24] and are shown in Figs. 2 and 3, and also in Figs. S-III–S-VIII of the Supplementary material.

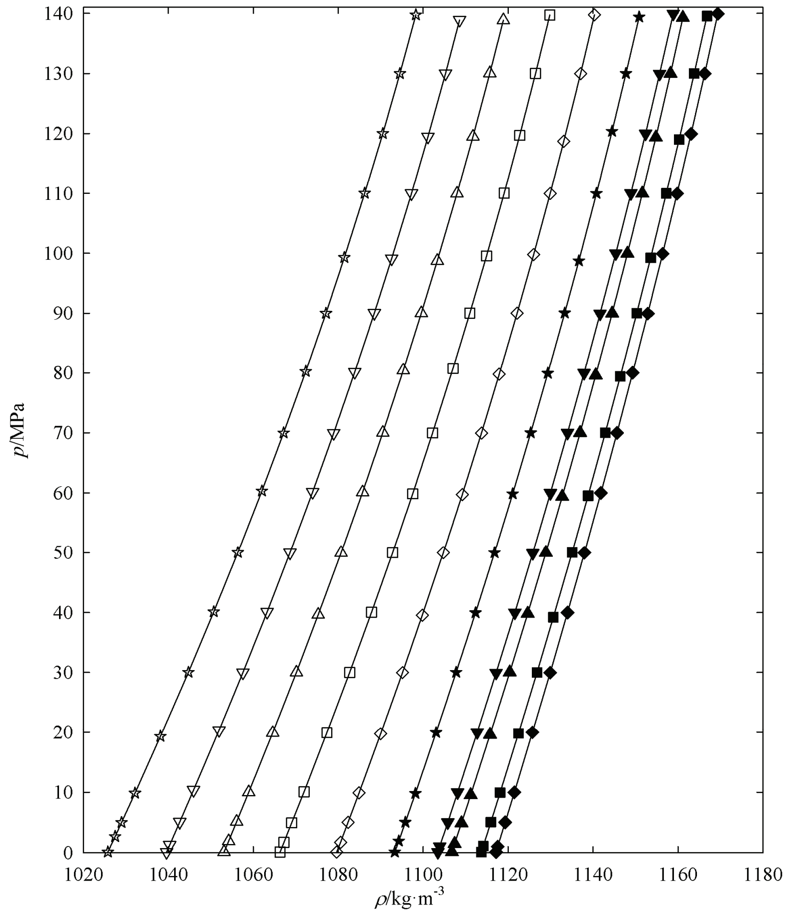

Fig. 1. Plot of pressure p of [OMIM][BF_4] *versus* density ρ: ◆, 278.15 K; ■, 283.15 K; ▲, 293.15 K; ▼, 298.15 K; ★, 313.16 K; ◇, 333.15 K; □, 353.15 K; △, 373.15 K; ▽, 393.14 K; ☆, 413.14 K; lines: calculated according to Eqs. (2)–(5).

The definition of $c_v(p_0,T)$ in Eq. (S-10) enables the calculation of $c_v(p,T)$ in Eq. (10) and $c_p(p,T)$ in Eq. (11) at high pressures and temperatures, whereas the density of [OMIM][BF_4] was experimentally investigated. The value of $c_v(p_0,T)$ can be calculated using the $c_p(p_0,T)$ values at ambient pressure and the data obtained at the experimental temperatures (p,ρ,T).[3] The calculated differences in specific heat capacities $c_p(p,T) - c_v(p,T)$ / J kg$^{-1}\cdot$K^{-1} at high pressures were used for the calculation of constant pressure heat capacity $c_p(p,T)$ in Eq. (S-11) (Supplementary material) at high pressures and temperatures.

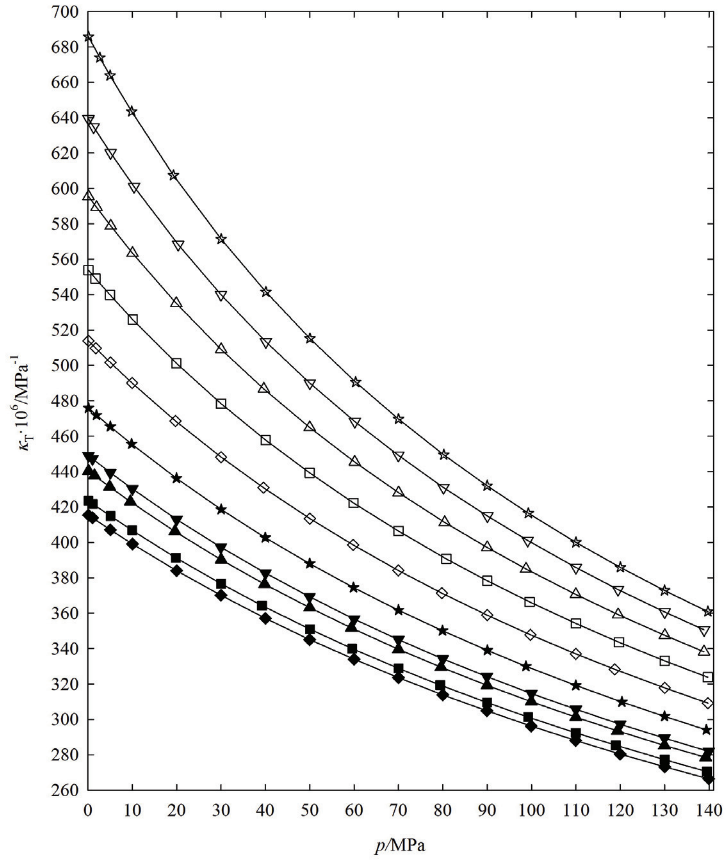

Fig. 2. Plot of isothermal compressibility $\kappa_T \cdot 10^6$ / MPa^{-1} of [OMIM][BF_4] *versus* pressure p: ◆, 278.15 K; ■, 283.15 K; ▲, 293.15 K; ▼, 298.15 K; ★, 313.16 K; ◇, 333.15 K; □, 353.16 K; △, 373.16 K; ▽, 393.14 K; ☆, 413.14 K; the lines are the best fit lines.

After determination of specific heat capacities of [OMIM][BF_4], it is possible to establish the speed of sound at high pressures and various temperatures $u(p,T)$ using the following thermodynamic equation:

$$u^2(p,T) = \frac{c_p(p,T)}{c_v(p,T)} \left(\frac{\partial p(T,\rho)}{\partial \rho} \right)_T \tag{8}$$

Furthermore, the isentropic exponent $\kappa_s(p,T)$ can be obtained using the following relation:

$$\kappa_{\mathrm{S}}(p,T)=\frac{\rho(p,T)}{p}\frac{c_p(p,T)}{c_V(p,T)}\left(\frac{\partial p(T,\rho)}{\partial \rho}\right)_T \tag{9}$$

The calculated values are also presented in Table S-II together with (p,ρ,T) data.

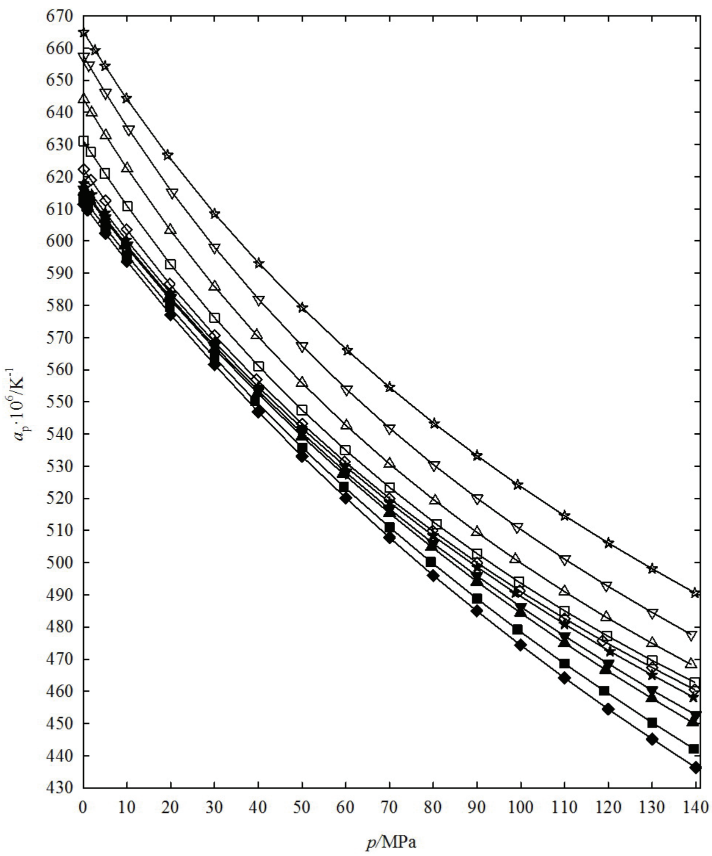

Fig. 3. Plot of isobaric thermal expansibility $\alpha_p\cdot10^6$ / K^{-1} of [OMIM][BF_4] *versus* pressure p: ◆, 278.15 K; ■, 283.15 K; ▲, 293.15 K; ▼, 298.15 K; ★, 313.16 K; ◇, 333.15 K; □, 353.16 K; △, 373.16 K; ▽, 393.14 K; ☆, 413.14 K; the lines are the best fit lines.

Most of the derived thermophysical properties increase with increasing temperature and decrease with increasing pressure. However, the thermal pressure coefficient and speed of sound increase with increasing pressure and decrease with decreasing temperature. The internal pressure values decrease with increasing temperature up to around 20 MPa and thereafter increase with increasing temperature. The values decrease with increasing pressure at around temperature T = 393.15 K and thereafter increase with increasing of pressure. This interesting behaviour could be explained as resulting from the existence of attractive forces under low-pressure conditions but as the pressure increases, repulsive forces become dominant at low temperatures for the IL. It was also observed that p_{int} increases with respect to temperature at a fixed pressure for $p > 20$ MPa for the IL. On the other hand, the internal pressure decreases with increasing temperature for normal liquids because an increase in temperature only affects the coordination number, while the intermolecular distances within the liquid molecules remain unchanged.[25] This behaviour might be related to the self-associated structure of the IL of the cationic part, or inherent structural heterogeneities of the polar and non-polar groups of the IL.[26]

The obtained values of specific heat capacities at constant pressure $c_p(p,T)$, constant volume $c_v(p,T)$ and speed of sound $u(p,T)$ at high pressures and temperatures were fitted to the double polynomial equation:

$$c_p(p,T) = \sum_{i=0}^{3} (p\,/\,\mathrm{MPa})^i \sum_{j=0}^{3} d_{ij}(T/K)^j \tag{10}$$

$$c_v(p,T) = \sum_{i=0}^{3} (p\,/\,\mathrm{MPa})^i \sum_{j=0}^{3} e_{ij}(T/K)^j \tag{11}$$

$$u(p,T) = \sum_{i=0}^{3} (p\,/\,\mathrm{MPa})^i \sum_{j=0}^{3} f_{ij}(T/K)^j \tag{12}$$

where d_{ij}, e_{ij} and f_{ij}, the coefficients of Eqs. (10)–(12), are presented in Tables S-IV–S-VI of the Supplementary material. The equations presented in this paper and its Supplementary material where used for fitting the experimental results, with *APD* values of $\Delta c_p/c_p$ = 0.016, $\Delta c_v/c_v$ = 0.058 and $\Delta u/u$ = 0.016 %, respectively.

DISCUSSION

The measured (p,ρ,T) data for [OMIM][BF_4] were analyzed and compared with the available literature values. The results of comparison are shown in Fig. 4. Eqs. (2)–(5) were used to interpolate the obtained results for similar temperature and pressure conditions as found in the literature.

The obtained high pressure–high temperature density values were compared with the available literature values (Table S-I). The thirteen density values for [OMIM][BF_4] out of fifteen measured by Gu and Brennecke[7] have a $\Delta\rho/\rho$ = = ±1.08 % *PD* deviation from the present values. The maximum *PD* value is $\Delta\rho/\rho$ = = 1.41 % at T = 298.2 K and p = 103.52 MPa. Seventy (p,ρ,T) data values of Harris *et al.*[8] out of eighty-one are mostly higher than the present results with $\Delta\rho/\rho$ = 0.08 % *APD*. The maximum *PD* of these literature values is $\Delta\rho/\rho$ = 0.39 % at T = 323.15 K and p = 125.5 MPa. The seventy seven (p,ρ,T) results for

[OMIM][BF_4] presented by Gardas *et al.*[9] were compared with our results and have PD in $\Delta\rho/\rho = \pm0.10$ %. The maximum PD of this comparison is $\Delta\rho/\rho = 0.18$ % at $T = 293.15$ K and $p = 0.101$ MPa. The one hundred nineteen (p,ρ,T) data of [OMIM][BF_4] measured by Sanmamed *et al.*[10] have $\Delta\rho/\rho = \pm0.11$ % *PD* from the present results with a $\Delta\rho/\rho = 0.17$ % maximum *PD* at $T = 283.15$ K and $p = 60$ MPa. The twenty (p,ρ,T) values of [OMIM][BF_4] determined by Tomida *et al.*[11] showed an *APD* in $\Delta\rho/\rho = 0.05$ % to present values with $\Delta\rho/\rho = 0.08$ % at $T = 293.15$ K and $p = 20$ MPa.

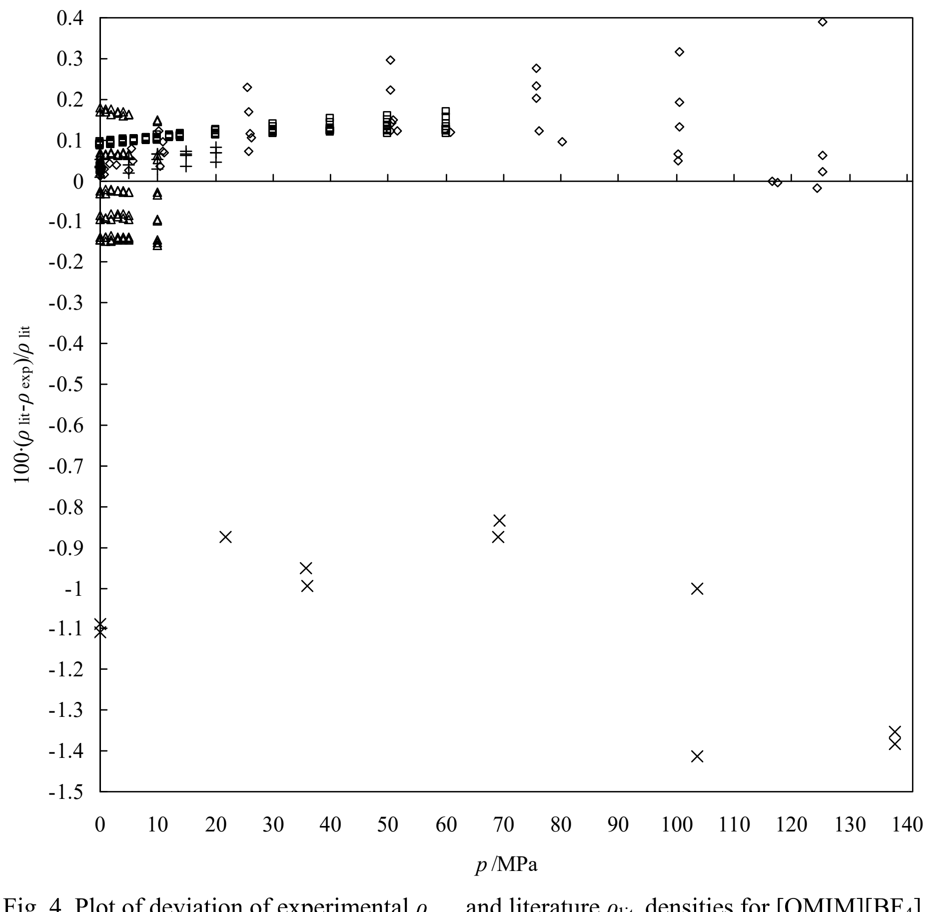

Fig. 4. Plot of deviation of experimental $\rho_{exp.}$ and literature $\rho_{lit.}$ densities for [OMIM][BF_4] *versus* pressure at various temperatures: ×, Gu and Brennecke;[7] ◇, Harris *et al.*;[8] △, Gardas *et al.*;[9] □, Sanmamed *et al.*[10] and +, Tomida *et al.*[11]

As the result of these comparisons, it could be seen that the present (p,ρ,T) results have low deviations from the values of Gardas *et al.*,[9] Sanmamed *et al.*[10]

and Tomida *et al.*[11] and the present results together with these literature values could be used for reference purposes in the future.

The eighty literature isobaric thermal expansibility α_p values of Navia *et al.*[25] were compared with the present calculated values and the *APD* in $\Delta\rho/\rho$ of 2.58 % was obtained.

Speed of sound $u(p_0,T)$ values calculated using Eq. (20) in 278.15–343.15 K range and p = 0.101 MPa were compared with values from a previous paper[3] and an *APD* of 1.8 % was obtained. This deviation can be attributed to uncertainties in the ambient pressure heat capacity $c_p(p_0,T)$ or ambient pressure thermal properties (isothermal compressibility κ_{T0}, isobaric thermal expansibility α_{p0}, difference in isobaric and isochoric heat capacities (c_p–c_v)) determined from experimental (p,ρ,T) values.

CONCLUSIONS

The thermophysical properties of [OMIM][BF_4] over a wide range of temperatures T and pressures p are reported. The measured (p,ρ,T) results of [OMIM][BF_4] were correlated with the equation of state developed by our group, which fitted extremely well with deviations from experimental data of ±0.011 %. All available density ρ values of [OMIM][BF_4] presented in the literature at various pressures and temperatures were compared with the obtained results and mostly the agreement was good. The experimental (p,ρ,T) results were also used to derive thermodynamic properties, such as isothermal compressibility, isobaric thermal expansibility, differences in isobaric and isochoric heat capacities, thermal pressure coefficient, internal pressure, heat capacities at constant pressure and volume, speed of sound and the isentropic exponent at temperatures from 278.15 to 413.15 K and pressures p up to 140 MPa. For this purpose, the combination of experimental values of density, isobaric heat capacity and speed of sound values at ambient pressure were also successfully established.

The obtained experimental and calculated results could be used for the application of [OMIM][BF_4] for various purposes, as discussed in the introduction to this paper.

List of symbols

p	Absolute pressure, Pa
T	Absolute temperature, K
p_{int}	Internal pressure, Pa
c_p	Isobaric heat capacity, J K^{-1}
c_v	Isochoric heat capacity, J K^{-1}
u	Speed of sound, m s^{-1}
PD	Percent deviation, %
APD	Average percent deviation, %

Greek letters

ρ Density, kg m^{-3}
κ_s Isentropic exponent
κ_T Isothermal compressibility
α_p Isobaric thermal expansibility
γ Thermal pressure coefficient

Index

0 Ambient pressure

SUPPLEMENTARY MATERIAL

Additional data and considerations are available electronically at the pages of the journal website: http://www.shd.org.rs/JSCS/, or from the corresponding author on request.

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ИЗВОД

(p,ρ,T) СВОЈСТВА 1-ОКТИЛ-3-МЕТИЛИМИДАЗОЛИЈУМ-ТЕТРАФЛУОРОБОРАТА

JAVID T. SAFAROV[1,2] AYGUL T. NAMAZOVA[2], ASTAN N. SHAHVERDIYEV[2] и EGON P. HASSEL[1]

[1]*Institute of Technical Thermodynamics, University of Rostock, Germany и* [2]*Department of Heat Energy, Azerbaijan Technical University, Baku, Azerbaijan*

У овом раду су приказани резултати експерименталног одређивања (p,ρ,T) података, у широком опсегу температура од 278,15 до 413,15 K и на притисцима до 140 MPa. Процењена вредност експерименталног средњег процентуалног одступања (*APD*) одређивања густине је ±0,01–0,08 %. Мерења су извршена помоћу Anton Paar DMA HPM густиномера са вибрирајућом капиларом. (p,ρ,T) подаци за [OMIM][BF_4] су фитовани, а параметри примењене једначине одређени као функција притиска и температуре. Након детаљне анализе литературних података и валидирања коришћене једначине стања, за испитивани систем, у температурном опсегу од 278,15 до 413,15 K и на притисцма до 140 MPa, израчуната су и друга термофизичка својства, као што су изотермска компресибилност, коефицијент изобарске експанзије, разлика у изобарском и изохорском топлотном капацитету, унутрашњи притисак, изобарски и изохорски топлотни капацитет, брзина звука, итд.

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