Comparative Study of Correlation for the Densities of Ionic Liquids

By

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Dissertation submitted in partial fulfillment of

the requirements for the

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(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the

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Approved by,

_____

(Assoc. Prof. Dr. Khashayar Nasrifar)

Universiti Teknologi PETRONAS

TRONOH, PERAK

May 2013

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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Abstract

This paper presents the comparative study of correlations as to estimate the densities of ionic liquids. The correlations used in this study are of generalized correlation and the one that is developed for the calculation of the density of saturated and normal liquid. 8 correlations are used in this study and the accuracy of the correlations is determined by calculating the deviations. The generalized models used in the estimation of ionic liquids density are Yamada and Gunn – YG (1973, pg. 234), Reid et al. – RR (1977), Bhirud – BH (1978, pg. 1127), Hankinson and Thomson – HT (1979, pg. 653), Valderrama and Abu Sharkh – VSY and VSD (1989, pg. 87), Mchaweh et al. – MH (2004, pg. 157) and Valderrama and Zarricueta – VZ (2009, pg. 145). In this paper, 139 density data of imidazolium based ionic liquids, 57 of ammonium based and 20 density data of pyridinium based ionic liquids are assembled to conduct the study. The best correlation to be used for the estimation of ionic liquids density is determined based on the lowest deviations calculated.

Acknowledgment

First of all, all praises be to Allah as for His willingness, I am able to complete the report and the project work. I would like to express my gratitude to Universiti Teknologi PETRONAS as in this course; I have the opportunity to be involved in managing a project on my own. This gives me the experiences of hectic deadlines and consequently challenges my problem solving and time management skills, which I believe will be useful in the future.

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ABBREVIATIONS AND NOMENCLATURES

List of symbols

T_r : Reduced temperature
T_{br} : Reduced base temperature
T_c : Critical temperature
T_b : Base temperature
V_c : Critical volume
M : Molecular weight
Gas constant, R = 0.083145

List of basic equations

$$T_r = \frac{T}{T_c}$$

$$T_{br} = \frac{T_b}{T_c}$$

$$\rho_c = \frac{1}{V_c} \times M$$

Greek Letters

ρ : Density
ρ_c : Critical density (M/V_c)
ρ_{lit} : Literature data of liquid density
ρ_{calc} : Calculated density of liquid
ω : Accentric factor
γ : Parameters in VSY model
τ : Parameters in Mchaweh model
δ : Parameters in Valderrama and Zarricueta model
Δ : Deviations

Abbreviations

BH Bhirud model
YG Yamada and Gunn model
HT Hankinson and Thomson model
LGM Linear generalized model
MH Mchaweh model
RR Reid et al. model
VSY Valderrama and Abu Sharkh model
VSD Valderrama and Abu Sharkh model
VZ Valderrama and Zarricueta model

CHAPTER 1

INTRODUCTION

1. INTRODUCTION

1.1 Background of Study

Ionic liquids are molten salts at room-temperature and they are entirely comprised of ions; cation and anion (Shen et al., 2011, pg. 2690). They melt at low temperature – generally below normal boiling point of temperature of water – and thus existed in liquid phase under room temperature. Due to that reason, most ionic liquids are known as room temperature ionic liquids (RTIL) (Pratap Singh & Kumar Singh, 2011, pg. 1).

Currently, chemical industries and scientific communities have given their attention on the opportunities to utilize ionic liquids in as much application, replacing the conventional solvents in chemical processes (Shen et al., 2011, pg. 2690). This is due to the unique properties possessed by the substance which include; 1) negligible vapor pressure, 2) non-flammable, 3) good thermal and chemical stability, 4) low toxicity, 5) miscible with various compounds covering wide range of polarity, and most importantly, 6) the ability to be molecularly tuned or engineered for any specific applications (Shen et al., 2011, pg. 2690), (Roshan & Ghader, 2012, pg. 33).

Abildskov et al. (2009, pg. 95) stated that ionic liquids can be used as chemical reaction media, separation process fluids and for processing of metals and

polymers and electrolytes in electronic devices. Other possible applications of ionic liquids are extraction of metal from waste water through emulsion, as electrolytes in lithium rechargeable batteries and super-capacitors and as thermal fluids for heat storage (Hosseini et al., 2012, pg. 52). Due to these advantages and wide applications, they become the researchers' focus and thus, knowing their properties becomes extremely important.

One of the important physical properties of a liquid is its density. As stated by Valderrama and Zarricueta (2009, pg. 145), liquid density is required in design problems, vessel sizing and liquid metering calculations. This property is usually measured experimentally and as for ionic liquids, there are many density data available as the result of the laboratory procedures for density identification of certain group of ionic liquids. However, due to the tunable properties of ionic liquids, lots of new ionic liquids are designed and hence, thousands of density data are required to be known. Due to this, the determination of density through experiments would be expensive and time consuming. Therefore, researchers need to come up with different method and that will be the estimation by using correlations.

Previous researchers had conducted various methods and developed several correlations in order to produce the most accurate result in estimating the density of ionic liquids. A group contribution method is one of the most practical choices in predicting the properties of ionic liquids. With the principle of assuming similar structures of chemical components in different molecules, chemical compounds are categorized based on the atoms and the bonds which then, a correlation can be developed. Thus, the properties of mixtures and pure components can be predicted by using the properties of the group or atom. Therefore, thousands of data on the properties of compounds would not be needed as knowing only hundreds of groups would be sufficient to estimate the properties of the constituents' compounds.

The example of a group contribution method is the study by Qiao et al. (2010). The paper presented the result of the density estimation based on 51 groups

of 123 pure ionic liquids with 13 binary ionic liquids mixtures, which shows the average relative error of 0.88% and the standard deviation of 0.0181.

Another commonly used method is through the developed correlations for the density estimation of ionic liquids. The correlations are basically generalized from the equations that are used for calculating the density of normal liquids. However, there are lacks of common basic data for ionic liquids, such as the critical temperature. As been stated in Valderrama and Zarricueta (2009), under low temperature, the ionic liquids start to decompose, especially at the temperatures approaching boiling point. This results in a failure to determine the critical properties of the ionic liquids. Therefore, under this circumstance, approximations of those properties are considered as reasonable option in order to estimate the density of ionic liquids. This is agreed by Qiao et al. (2010, pg. 852) which commands the necessities to estimate the properties of the compounds.

One of the previous studies which developed a generalized model for estimation of ionic liquids density is by Valderrama and Zarricueta (2009). The study had developed a model which considers much detail aspects of ionic liquids in order to yield more accurate results. The model includes the critical temperature, critical volume, normal boiling point and the molecular mass for the estimation of the density. The result shows that the model yields a low average deviation, which is 2.6% and can be applied for the estimation of ionic liquids density.

There are a lot of previous studies that presented the work in estimating the density of ionic liquids. However, these studies were only conducted on certain ionic liquids and do not provide much database in predicting the density of ionic liquids. For example, the study by Valderrama and Zarricueta itself was considering only 146 ionic liquids from various groups of cations. Roshan and Ghader (2012, pg. 33) conducted the study for only 48 ionic liquids which comprised of random groups of cations, but mostly of imidazolium cation. Therefore, this study will estimate the density of another 216 ionic liquids – 139 of imidazolium-based, 57 ammonium-based and 20 pyridinium-based ionic liquids.

Through this study, this paper will present 8 correlations that are studied comparatively in order to determine the best correlations to be used to determine the density of ionic liquids. The selected correlations, except of Valderrama and Zarricueta, have not yet been applied for predicting density of ionic liquids. The accuracy of the correlations will be determined through the determination of absolute percent deviation for the calculated density of individual ionic liquids.

1.2 Problem Statement

According to the authors of previous papers, the density of ionic liquids can be estimated via correlations and yet, there are numbers of correlations developed for predicting the densities of normal liquids. However, the correlations could not be simply applied to estimate the density of ionic liquids, as critical properties are required for the estimation.

As been mentioned in the previous sub-chapter, the critical properties of ionic liquids could not be determined experimentally. Due to that reason, there are only few records on the correlations for calculating the density of ionic liquids. This leads researchers to developed correlations from various methods including the group contribution method and generalized models for the estimation of the density of ionic liquids.

It is stated that a good approximation values of the critical properties can be considered in order to apply the correlations of normal liquids for predicting the density of ionic liquids. Therefore, the accuracy of the correlations needs to be calculated. In this study, the most appropriate correlations will be selected among the 8 that are selected as the focus of this study.

1.3 Objectives

The main objective of this study is to determine the accuracy of the generalized correlations of liquid density in the estimation of the density of ionic liquids through calculation of relative and absolute percent deviations. It is essential to determine the density of ionic liquids via generalized correlations since there are some of the compounds that do not acquire any experimental data. Therefore, by determining the accuracy based on the experimental and the calculated density data, the best correlations can be highlighted and can be utilized for the estimation of the density of ionic liquids.

1.4 Scope of Study

In this project, the scope of study coverage is listed as follows:

- The assembled of ionic liquid density data of imidazolium-, ammonium- and pyridinium-based in different temperature range
- Finding at least 7 generalized density correlations available in the literature for the estimation of ionic liquid density
- Identifying the critical properties of ionic liquids (T_b, T_c, P_c, V_c, ω, etc.) and the required parameters based on the collected correlations
- Calculation of relative and absolute percent deviations of calculated density and the experimental data for determining the accuracy of the correlations used

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

As been mentioned in the previous chapter, researchers have come up with generalized correlations for estimating the density of ionic liquids. However, the existing correlations for calculating the density of normal liquids are expected to be possible for the estimation of ionic liquids density, by approximating the critical properties of the ionic liquids. Therefore, this study will be focusing on determining the accuracy of the correlations by calculating the percent deviations and hence, selecting the best correlations that yield the lowest deviations among others.

In this chapter, the studies done by previous authors will be presented as to give an overview on the project work. Afterwards, the problems addressed in the previous chapter will be further explained and the solutions to overcome the problems will be highlighted with accordance to the referred papers.

2.2 Valderrama and Zarricueta (2009)

The study conducted is basically determining the best correlations for estimating the density of ionic liquids. The previous work that has the closest similarity by which becoming the main reference for this project is the study by Valderrama and

Zarricueta (2009). In the paper, a simple model is developed for predicting the density of ionic liquids.

The model is a generalized correlation which is modified and includes the use of experimental data that is used to fit the parameters. The model also uses the critical temperature, critical volume, normal boiling temperature and the molecular mass as to estimate the density of ionic liquids. The correlation, which is named as Linear Generalized Model (LGM) is presented below:

$$\rho = \left(\frac{A}{B}\right) + \left(\frac{2}{7}\right) . \left\{\frac{A \ln B}{B}\right\} \frac{(T - T_b)}{(T_c - T_b)}$$

Where,

$$A = a + b.\frac{M}{V_c}$$

$$B = \left(\frac{c}{V_c} + \frac{d}{M}\right) . V_c^{\delta}$$

The constants a, b, c, d and δ were determined in the study using the literature density data of ionic liquids and valid for any ionic liquid for future studies; where, a = 0.3411; b = 2.0443; c = 0.5386; d = 0.0393; δ = 1.0476. In the study, Valderrama and Zarricueta had selected 146 random ionic liquids with 602 density data as their main focus. The calculated density is then compared with the literature density data of the respective ionic liquids to determine the percent deviations. The generalized model is studied comparatively with other 10 correlations which are used for the estimation of normal liquids density.

From the study, the deviations for each applied correlation is calculated and compared as to determine which correlation resulted in the lowest percentage. The result of the study shows that the LGM yield the average absolute percent deviation of 2.6% which is the lowest compared to others. The paper had proven that the generalized model can be used confidently in estimating the density of any ionic

liquids. This is most probably due to the used of the constants obtained from the literature density data which provides the validity for the applications of other ionic liquids. Therefore, in the study, for 146 ionic liquids, it is presented that the best correlation would be the LGM.

2.3 Other Studies

There are various studies that have been conducted as to develop generalized correlations for estimating the density of ionic liquids. The following examples are the few studies that were done previously based on different methods. Nevertheless, the studies share the same goal; to develop an accurate correlation for predicting the density of ionic liquid.

2.3.1 Gardas and Coutinho (2008)

In the study done by Gardas and Coutinho (2008, pg. 26), the estimation of densities of ionic liquids is basically the extension of the Ye and Shreeve group contribution method. Ye and Shreeve (2007) had proposed a method for the estimation of ionic liquids densities based on group additivity and calculated volume parameters of groups and fragments for the stated estimation. Although, the model is reported to be simple, the method is not straightforward.

The extension studies had tested to estimate the density of ionic liquids in wide ranges of temperature and pressure using the proposed parameter table from Ye and Shreeve (2007). The coefficients of the new density correlation were estimated using experimental densities data of nine ionic liquids which are of imidazolium, pyridinium, pyrrolidinium and phosphonium cations.

$$\rho = \frac{W}{NV_o(a + bT + cP)}$$

Shown above is the correlations used by Gardas and Coutinho in order to determine the density of ionic liquids. The coefficients a, b and c can be estimated by fitting the equations with experimental data, W is the molar mass (kg/mol^{-1}), N is the Avogadro constant and V_0 (m^3) molecular volume at the reference temperature, T_0 and pressure, P_0. Based on the studies, the prediction are considered successful with experimental literature data in a wide range of temperatures (273.15-393.15 K) and pressures (0.10-100 MPa) with the mean percentage deviation (MPD) of 0.45% for imidazolium-based ionic liquids, 1.49% for phosphonium-based ionic liquids, 0.41% for pyridinium-based and 1.57% for pyrrolidinium-based ionic liquids.

2.3.2 Chong Shen et al. (2011)

Other studies had also been conducted on the prediction of ionic liquids densities and some had presented the extension studies done by the previous researchers as to obtain further results on the prediction of ionic liquids densities. Chong Shen, et al. (2011, pg. 2690) had extended the group contribution model by Valderrama and Robles into the prediction of densities and critical properties of ionic liquids at varying temperatures and pressures. Shown below is the correlation used in the study.

$$\rho = \frac{M}{V_m} = \frac{pM}{ZRT}$$

As seen above, the correlation is simple and does not require any complex calculations.

2.3.3 Valderrama and Rojas (2010)

Valderrama and Rojas (2010, pg. 107) had proposed a general model for the density estimation based on the concept that was first introduced by Randic (1975). The new proposed concept is reported to be much easier to calculate than any of the connectivity indexes available in the literature. The correlation is defined as follows.

$$\rho = \rho_0 - (3.119 \times 10^{-3})\lambda(T - T_0)$$

Where ρ_0 is the density at T_0 = 298 K and λ is the mass connectivity index of the ionic liquids.

2.4 Summary

Presented above are few examples of developed and generalized correlations for the estimation of ionic liquid density. The correlations had been tested and the results give a feasible value of deviation, which is then agreed to have a good capability to estimate the density of ionic liquids.

However, it has been a wonder for researchers whether a correlation for estimating the density of pure and normal liquids is applicable for that of ionic liquids. The previous authors were then interested to carry out studies to determine the accuracy of the correlations. The studies were carried out on different type and groups of ionic liquids. As known, ionic liquid is a unique solvent which can be engineered and thus, newly developed ionic liquids are produced day by day.

Therefore, this study is carried out on another 214 ionic liquids which is collected from Lazzus (2009) and the focus would be on -imidazolium, -ammonium and –pyridinium based ionic liquids. This study is a continuation from Valderrama and Zarricueta (2009), which a target is set – to determine the best correlation and calculating the deviations for each of selected ionic liquid.

CHAPTER 3
METHODOLOGY

3.1 Project Methodology

Generally, the methodology for the project is the analysis and reviews of previous studies and literatures. Specifically, the sequence of the project work is as shown in the diagram below.

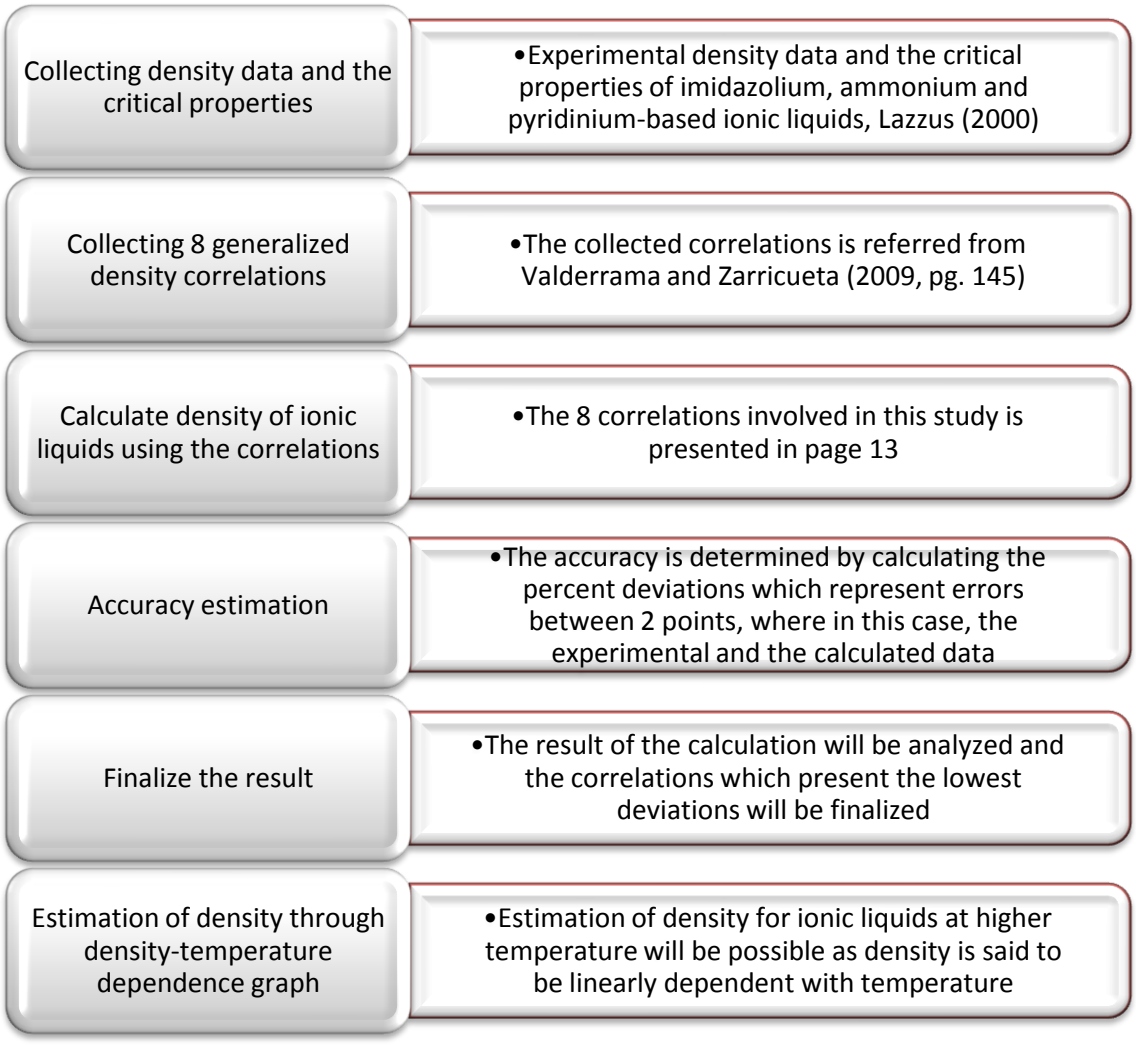


Figure 3.1: Project Methodology Flowchart

3.2 Selected Correlations for the Study

The generalized correlations for the estimation of ionic liquids density used in this study is as presented as follows.

Table 3.1: Model of Generalized Correlations

Model	Equation
Yamada and Gunn (T_c, V_c, M, ω)	$\rho = \rho_c(0.29056 - 0.08775\omega)^{-(1-T_r)^{2/7}}$
Reid et al. (T_c, V_c, M, ω)	$\rho = \rho_c[1 + 0.85(1 - T_r) + (1.6916 + 0.984\omega)(1 - T_r)^{\frac{1}{3}}]$
Bhirud (T_c, P_c, M, ω)	$ln\frac{P_c}{\rho RT} = ln\, V^{(0)} + \omega\, ln\, V^{(1)}$ $ln\, V^{(0)} = 1.39644 - 24.076T_r + 102.615{T_r}^2 - 255.719{T_r}^3 + 355.805{T_r}^4 - 256.671{T_r}^5 + 75.1088{T_r}^6$ $ln\, V^{(1)} = 13.4412 - 135.7437T_r + 533.380{T_r}^2 - 1091.453{T_r}^3 + 1231.43{T_r}^4 - 728.227{T_r}^5 + 176.7377{T_r}^6$
Hankinson and Thompson (T_c, V_c, M, ω)	$\rho = \frac{\rho_c}{[\, V^{(0)}(1 - \omega\, V^{(1)}]}$ $V^{(0)} = 1 - 1.5281(1 - T_r)^{1/3} + 1.4390(1 - T_r)^{2/3} - 0.8144(1 - T_r) + 0.19045(1 - T_r)^{4/3}$ $V^{(1)} = \frac{(-0.296123 + 0.386914T_r - 0.0427258{T_r}^2 - 0.0480645{T_r}^3)}{(T_r - 1.00001)}$
Valderrama and Abu Sharkh (VSY) (T_c, V_c, M, T_b)	$\rho = \left(0.01256 + 0.9533\frac{M}{V_c}\right)[\left(\frac{0.0039}{M} + \frac{0.2987}{V_c}\right){V_c}^{1.033}]^{\gamma(T)}$ $\gamma(T) = -[\frac{(1 - T_r)}{(1 - T_{br})}]^{2/7}$
Valderrama and Abu Sharkh (VSD) (T_c, P_c, V_c, M, T_b)	$\rho = \left(\frac{MP_c}{RT_c}\right)\left[\left(0.3445\frac{P_c}{RT_c}\right){V_c}^{1.0135}\right]^{-\frac{[1+(1-T_r)^{\frac{2}{7}}]}{[1+(1-T_{br})^{\frac{2}{7}}]}}$
Mchaweh et al. (T_c, V_c, M, ω)	$\rho(T) = \rho_c(1 + 1.169\tau^{\frac{1}{3}} + 1.818\tau^{\frac{2}{3}} - 2.658\tau + 2.161\tau^{\frac{4}{3}})$ $\tau = 1 - \frac{\left(\frac{T}{T_c}\right)}{[1 + m(1 - \sqrt{T/T_c})]^2}$ $m = 0.480 + 1.574\omega - 0.176\omega^2$

Valderrama and Zarricueta (T_c, T_b, V_c, M)	$\rho = \left(\frac{A}{B}\right) + \left(\frac{2}{7}\right).\left\{\frac{A.\ln B}{B}\right\}.\frac{(T - T_b)}{(T_c - T_b)}$ $A = a + b.\frac{M}{V_c}$ $B = \left(\frac{c}{V_c} + \frac{d}{M}\right).V_c^{\delta}$ a = 0.3411; b = 2.0443; c = 0.5386; d = 0.0393; δ = 1.0476

The deviations are calculated using the following equation.

Average relative percent deviation,

$$\%\Delta\rho = \frac{100}{N}\sum\left[\frac{\rho^{lit} - \rho^{cal}}{\rho^{lit}}\right]$$

Average absolute percent deviation,

$$|\%\Delta\rho| = \frac{100}{N}\sum\left|\frac{\rho^{lit} - \rho^{cal}}{\rho^{lit}}\right|$$

Based on the generalized correlations, the estimated density of ionic liquids and the deviations is calculated as to determine the approximate error of each of the presented model. The result is as shown in the following chapter.

CHAPTER 4

RESULTS AND DISCUSSION

The 216 ionic liquids which are of imidazolium, pyridinium and ammonium based cations are arranged and the calculated density is determined. The project fully utilized Microsoft Excel as to calculate the estimated density. The spreadsheet of the calculation, together with the properties and important values of the selected ionic liquids is presented in the Appendix.

4.1 Average Absolute Percent Deviation – Result

The following table presents the deviations between the experimental density data of ionic liquids and the estimated density, calculated from the generalized models, the average absolute percent deviation with the minimum and maximum values calculated from individual ionic liquids.

Table 4.1: Average absolute percent deviation, $|\%\Delta\rho|$

Cation	YG	RR	Bhirud	HT	VSY	VSD	MH	VZ
Imidazolium	5.81	4.65	56.82	5.46	5.15	55.43	6.58	3.09
Ammonium	12.45	9.41	131.22	11.86	7.36	58.42	4.43	3.73
Pyridinium	6.09	5.13	69.18	5.88	5.33	54.11	5.93	2.81
Total Average	**7.58**	**5.94**	**77.48**	**7.18**	**5.75**	**56.10**	**5.96**	**3.23**
$\|\%\Delta\rho\|_{min}$	**0.05**	**0.00**	**0.48**	**0.01**	**0.17**	**31.97**	**0.06**	**0.00**
$\|\%\Delta\rho\|_{max}$	**46.04**	**26.27**	**4129.8**	**40.68**	**23.23**	**69.98**	**26.00**	**25.21**

Referring to Table 4.1, it is shown that Valderrama and Zarricueta model represent the lowest average absolute percent deviations. Table 4.2, 4.3 and 4.4 shows the deviation of the ionic liquids, individually.

Table 4.2: Deviations of experimental data and calculated density of imidazolium based ionic liquids

Abbreviation	YG	RR	Bhirud	HT	VSY	VSD	MH	VZ
[mim][Cl]	1.83	1.46	15.78	2.25	5.67	31.97	5.50	13.54
[emim][tsac]	4.31	4.13	12.27	4.26	0.33	55.82	4.11	1.37
[bmim][TFES]	2.37	2.50	3.87	2.34	1.78	54.85	4.66	1.89
[dmim][TFES]	19.31	15.17	151.44	18.64	10.13	61.59	0.70	3.89
[emim][TFES]	7.40	6.81	6.02	7.33	10.54	55.65	11.79	5.19
[hpmim][TFES]	4.83	3.83	17.02	4.62	0.68	59.09	6.11	0.50
[bmim][HFPS]	2.22	2.08	12.55	2.14	1.38	56.74	5.74	0.06
[bmim][TPES]	9.86	9.22	15.59	9.70	6.28	56.13	0.39	4.66
[bmim][TTES]	6.96	6.68	4.82	6.87	3.07	55.58	1.91	3.59
[bmim][FS]	7.89	7.26	17.10	7.73	4.37	56.92	2.17	2.79
[bmim][Ac]	3.69	2.19	7.66	3.09	2.77	55.44	7.64	3.29
[emim][Ac]	6.74	6.00	20.12	6.25	1.02	49.52	2.49	10.50
[emim][BEI]	0.69	1.80	92.41	1.02	0.80	54.69	2.91	0.14
[bmim][BEI]	4.20	4.82	15.37	4.39	2.16	55.78	1.71	1.63
[dmprim][bti]	0.64	1.60	50.73	0.96	2.77	55.66	3.88	0.38
[dmprim][bti]	1.15	0.22	62.92	0.85	4.50	56.26	5.56	2.05
[dbim][bti]	4.41	4.17	30.12	4.23	8.34	61.70	11.45	8.58
[E1,3M4I][bti]	2.38	3.35	53.33	2.70	1.09	54.90	2.23	1.34
[dmim][bti]	5.49	3.98	41.43	5.03	7.58	51.99	5.80	1.69
[decmim][bti]	12.25	11.19	30.38	12.25	6.22	59.84	0.30	2.48
[hpmim][bti]	6.04	6.31	44.35	6.24	1.68	57.51	1.77	1.42
[nmim][bti]	9.70	9.15	35.06	9.77	4.29	59.25	1.14	1.75
[pmim][bti]	2.62	3.47	52.07	2.91	0.91	55.68	2.53	0.93
[prmim][bti]	0.42	0.83	58.59	0.04	3.30	53.69	3.30	0.46
[dmeim][bti]	1.44	0.18	65.91	1.06	4.34	53.70	4.10	0.26
[dmeim][bti]	2.79	1.53	57.89	2.42	5.49	54.49	5.31	1.54
[eomim][bti]	0.98	2.19	35.88	1.35	1.95	53.70	2.29	1.14
[Ph(CH2)mim][bti]	1.15	0.31	1.81	0.66	3.54	54.52	3.32	0.74
[Ph(CH2)2mim][bti]	0.67	0.62	5.03	0.22	3.31	55.90	3.90	1.45
[Ph(CH2)3mim][bti]	0.34	0.74	8.54	0.06	3.26	57.31	4.68	2.37
[bdmim][bti]	2.26	2.97	56.91	2.53	1.51	56.46	3.45	0.03
[C12mim][bti]	15.41	13.17	9.26	15.28	8.10	61.83	0.62	1.82
[memim][bti]	1.24	2.54	70.43	1.63	1.73	52.44	1.49	2.45
[mmim][bti]	2.54	1.06	52.02	2.10	4.97	51.44	3.56	0.46
[pdmim][bti]	0.64	1.60	50.73	0.96	2.77	55.66	3.88	0.38
[C2F3mim][bti]	1.57	0.12	89.03	1.15	3.12	51.59	2.82	0.67

[bmim][Br]	1.11	1.12	5.93	1.35	5.16	51.59	7.57	2.47
[moeemim][Cl]	4.29	3.64	2.87	3.91	0.55	52.91	4.74	5.61
[bmim][Cl]	3.58	3.57	1.14	3.86	7.14	51.47	9.60	3.00
[hmim][Cl]	1.26	0.65	2.22	0.85	3.32	53.77	7.29	4.09
[omim][Cl]	5.50	4.05	3.60	4.94	0.21	56.14	5.92	4.24
[Bemim][Cl]	2.60	2.83	11.47	2.80	7.10	55.43	10.10	0.50
[C12mim][Cl]	24.57	20.40	13.42	23.55	15.34	56.45	4.87	13.56
[emim][Cl]	10.55	10.17	7.18	10.72	13.25	50.62	14.51	1.20
[mmim][Cl]	5.51	4.96	19.16	5.66	8.08	44.63	8.87	6.34
[ClBenmim][Cl]	0.75	0.19	11.39	0.53	4.35	56.20	8.22	0.09
[FBenMim][Cl]	3.24	3.84	1.46	3.53	8.07	57.09	11.84	3.01
[dbim][Cl]	3.94	2.93	2.70	3.45	1.21	54.75	6.05	4.77
[bmim][dca]	9.09	4.98	97.03	8.26	1.76	61.18	9.49	0.59
[emim][dca]	8.26	5.28	87.34	7.58	1.53	58.15	7.63	2.52
[omim][dca]	15.10	8.74	160.03	13.97	2.15	64.02	8.66	1.58
[emim][dca]	8.26	5.28	87.34	7.58	1.53	58.15	7.63	2.52
[emim][DEGlyMSO4]	5.81	5.42	146.55	5.79	0.39	56.88	3.70	2.25
[dmim][DMPO4]	2.59	2.44	3.39	2.34	1.73	51.21	4.74	5.23
[edmim][ESO4]	0.14	0.16	10.56	0.22	5.50	51.64	5.90	2.79
[emim][ESO4]	0.74	0.11	82.18	0.62	5.68	53.15	5.77	2.06
[moim][PF6]	6.54	2.22	43.14	5.18	1.24	61.94	11.21	3.38
[moeemim][PF6]	12.94	8.95	40.43	11.62	5.00	57.38	4.63	3.91
[bdmim][PF6]	10.70	7.16	38.79	9.38	3.27	56.38	5.51	4.06
[hpmim][PF6]	7.55	3.25	42.36	6.16	0.43	60.73	10.17	1.90
[nmim][PF6]	12.33	6.67	39.90	10.74	3.04	62.33	8.70	1.15
[oprim][PF6]	21.94	15.23	34.37	20.17	11.45	60.59	2.07	5.58
[pmim][PF6]	2.14	0.87	43.00	0.99	4.36	59.29	12.26	3.35
[eommim][PF6]	2.84	0.62	43.43	1.81	2.89	55.58	9.67	0.10
[mommim][PF6]	1.74	3.38	45.30	2.64	6.65	55.09	12.41	2.63
[Ph(CH2)3mim][PF6]	2.08	0.98	38.16	1.20	4.47	62.36	13.03	6.19
[prmim][PF6]	3.01	1.03	40.39	2.01	2.40	54.38	8.85	1.45
[C2C6I][PF6]	7.53	3.23	42.37	6.14	0.44	60.74	10.19	1.92
[C2C8I][PF6]	12.35	6.69	39.89	10.76	3.05	62.32	8.68	1.14
[bmim][HSO4]	6.47	4.21	233.90	6.06	4.95	59.25	7.99	1.00
[emim][HSO4]	3.09	1.62	229.11	2.79	7.61	57.69	9.02	1.67
[mim][HSO4]	11.82	9.38	330.05	11.27	2.51	53.88	3.22	4.65
[bmim][I]	4.70	4.71	15.19	4.50	0.72	49.82	2.25	6.33
[bmim][mesy]	1.40	0.90	4.00	1.48	6.37	49.04	5.92	4.27
[emim][mesy]	4.84	4.02	87.22	4.69	9.47	52.56	8.56	0.16
[dmim][MOESO4]	1.72	1.16	80.86	1.60	6.61	54.40	7.06	0.00
[dmim][MSO4]	3.63	2.71	93.70	3.44	8.19	51.09	6.97	1.36
[bmim][MSO4]	0.20	0.62	80.70	0.28	4.99	54.43	5.81	1.69
[bmim][NfO]	5.97	5.65	28.41	5.86	3.46	56.61	2.89	2.21

[omim][NfO]	12.47	10.61	5.67	12.12	8.24	59.78	1.46	2.99
[bmim][C8S]	21.92	19.20	378.40	21.53	12.53	57.54	4.74	10.53
[moeoemim][BF4]	16.45	11.22	25.49	14.57	5.09	55.10	3.51	6.82
[bdmim][BF4]	16.56	11.92	19.87	14.63	5.75	51.83	1.91	10.41
[dmim][BF4]	24.00	15.83	24.13	21.63	9.96	59.64	2.37	6.66
[prmim][BF4]	1.81	0.75	23.82	0.39	6.03	51.62	10.94	1.83
[moemim][BF4]	7.26	4.14	23.73	5.74	1.46	51.54	7.23	4.83
[mommim][BF4]	2.54	0.13	24.82	1.18	5.18	50.50	9.92	2.53
[bmim][tca]	16.43	16.45	7.67	16.46	18.44	63.68	22.68	14.09
[emim][SCN]	21.86	21.45	0.48	21.81	23.15	63.15	26.00	16.50
[emim][ta]	8.83	9.27	29.49	9.24	12.45	56.19	15.99	6.20
[mpmi][TfO]	9.19	9.39	29.50	9.24	4.28	52.09	1.61	7.53
[dbim][TfO]	0.64	1.08	12.97	0.76	5.52	59.15	9.46	3.48
[Bemim][TfO]	6.79	7.23	66.73	6.91	2.30	52.86	0.13	6.10
[omim][TfO]	15.40	14.43	48.79	15.21	9.23	54.72	3.65	10.07
[dmpim][TMEM]	4.89	3.24	24.92	4.32	6.11	56.02	5.79	4.59
[bmim][TMEM]	3.51	1.78	22.98	2.92	4.59	54.83	3.98	2.74
[bmim][BF4]	0.18	2.78	26.45	1.55	7.85	54.16	12.93	0.84
[emim][BF4]	2.31	3.85	21.40	3.46	8.68	48.92	12.25	1.65
[hmim][BF4]	5.92	1.93	27.78	4.28	3.43	56.97	10.48	0.37
[omim][BF4]	12.60	7.23	31.68	10.59	1.54	57.33	7.11	3.26
[beim][bti]	0.05	0.97	37.56	0.28	3.11	56.09	4.24	0.80
[bmim][bti]	1.03	0.18	40.04	0.66	3.81	54.89	4.13	0.51
[deim][bti]	1.55	0.19	42.47	1.14	4.09	53.45	3.65	0.18
[dmeim][bti]	2.74	1.48	57.89	2.37	5.45	54.47	5.27	1.50
[dmim][bti]	5.54	4.04	55.94	5.09	7.63	51.86	5.83	1.67
[edmim][bti]	3.60	2.35	45.15	3.22	6.28	55.02	6.13	2.44
[eDmim][bti]	1.96	0.69	47.62	1.58	4.69	54.26	4.53	0.79
[emim][bti]	4.66	3.22	40.57	4.23	6.92	53.26	5.80	1.88
[hmim][bti]	2.24	3.03	1526.31	2.49	1.19	55.90	2.98	0.62
[ibmim][bti]	1.22	0.05	33.54	0.83	3.85	54.55	3.96	0.34
[mdeim][bti]	0.42	0.70	45.63	0.07	3.43	55.21	4.05	0.46
[meim][bti]	5.09	3.66	51.00	4.66	7.34	53.32	6.20	2.24
[moemim][bti]	5.85	4.53	16.81	5.45	7.90	55.73	7.86	4.16
[omim][bti]	5.23	5.41	127.45	5.37	0.98	57.90	2.62	0.62
[tfemim][bti]	5.44	4.09	42.99	5.05	6.81	54.26	6.89	3.50
[omim][Cl]	1.01	0.02	7.72	0.54	3.95	56.99	8.90	1.17
[emim][EtSO4]	3.90	3.11	48.48	3.76	8.27	52.64	7.73	0.54
[bmim][hb]	28.87	26.27	33.48	27.95	23.23	49.04	12.95	22.23
[emim][hb	2.10	0.97	47.58	1.52	1.29	55.57	7.92	0.40
[beim][MsO]	2.77	2.28	66.36	2.68	7.56	55.66	8.23	0.41
[emim][MsO]	8.27	7.34	78.43	8.08	12.37	53.25	11.07	2.29
[beim][NfO]	5.67	5.26	27.06	5.55	3.16	57.61	3.50	1.41
[emim][NfO]	5.22	4.91	32.56	5.10	2.91	56.92	3.51	1.72

[bmim][NO3]	4.86	5.75	8.97	5.23	10.58	58.38	14.13	4.55
[bmim][PF6]	3.98	5.75	48.58	4.97	8.98	56.55	14.71	4.70
[emim][PF6]	6.49	7.48	45.03	7.26	10.39	54.19	14.95	4.25
[hmim][PF6]	2.55	0.52	44.04	1.38	3.95	59.78	12.03	3.33
[omim][PF6]	7.57	3.36	46.83	6.12	0.24	60.33	9.85	1.53
[beim][ta]	5.60	3.81	21.30	4.92	0.17	56.51	6.61	2.56
[bmim][ta]	3.54	2.24	22.00	2.95	1.57	55.26	7.13	2.50
[deim][ta]	0.72	0.14	22.86	0.21	3.76	54.27	8.44	1.58
[emim][ta]	1.08	1.57	22.41	1.51	5.00	52.77	8.91	1.60
[beim][TfO]	0.07	0.36	16.86	0.01	3.83	54.97	5.86	0.95
[bmim][TfO]	1.45	0.80	11.56	1.35	4.87	53.56	6.10	1.10
[deim][TfO]	2.42	1.58	15.14	2.28	5.56	52.35	6.12	1.34
[doeim][TfO]	15.79	12.50	231.95	15.29	7.63	61.81	2.11	2.51
[edmim][TfO]	1.83	1.08	16.40	1.71	5.20	52.72	6.04	1.35
[emim][TfO]	5.13	4.16	11.99	4.96	7.95	51.58	7.84	0.10

Table 4.3: Deviations of experimental data and calculated density of ammonium based ionic liquids

Abbreviation	YG	RR	Bhirud	HT	VSY	VSD	MH	VZ
[TEA][tsac]	3.48	1.96	28.80	2.97	2.18	59.10	8.14	1.91
[TMAlA][tsac]	4.10	3.63	27.13	3.78	0.45	54.22	4.42	2.71
[TMEA][tsac]	3.22	2.94	28.58	2.93	0.98	53.16	4.54	2.96
[TMiPA][tsac]	1.27	0.76	30.23	0.94	3.09	55.77	7.18	0.24
[TMPA][tsac]	3.76	3.11	28.86	3.39	0.92	55.07	5.29	1.80
[NH221][BEI]	0.36	1.10	24.69	0.50	1.84	54.97	4.20	0.03
[NH11(i-3)][BEI]	0.96	0.22	25.68	0.81	3.12	55.56	5.45	1.33
[C27guan][bti]	22.05	13.43	47.56	21.14	10.88	69.98	7.66	7.16
[C15guan][bti]	7.42	3.93	176.87	6.98	0.90	66.44	10.41	7.84
[N723'3'][bti]	9.23	7.27	217.75	8.97	2.89	62.68	5.03	1.85
[BNM2E][bti]	1.77	2.39	1.38	1.89	1.57	54.99	3.49	1.36
[N1123][bti]	0.36	0.48	3.38	0.19	3.32	54.10	4.43	0.63
[N1134][bti]	3.51	3.87	7.51	3.59	0.23	56.04	3.02	1.60
[tda][bti]	9.02	8.91	67.83	9.39	13.38	64.99	1.45	3.38
[thpa][bti]	29.40	20.84	26.23	28.44	18.49	67.62	0.93	0.24
[tha][bti]	30.48	22.12	40.26	29.42	18.22	66.17	0.63	2.26
[tpa][bti]	23.53	17.58	273.53	22.72	12.99	64.87	0.89	1.55
[toa][bti]	27.35	20.79	53.11	26.77	20.58	67.06	0.59	0.29
[N7444][bti]	22.11	16.84	251.90	21.40	12.15	64.39	0.85	1.73
[N6444][bti]	23.55	18.89	473.44	22.92	14.03	62.80	1.74	4.59
[N1444][bti]	9.47	8.20	51.86	9.27	3.69	60.19	2.82	0.93
[N8444][bti]	28.21	22.01	171.41	27.39	17.26	63.75	2.74	5.21
[N7222][bti]	10.18	8.89	73.76	9.99	4.35	60.13	2.27	1.45

[N6222][bti]	9.09	8.29	46.66	8.98	3.82	58.93	1.83	2.13
[N8222][bti]	11.41	9.57	120.08	11.14	4.99	61.23	2.63	0.87
[N8222][bti]	8.56	6.79	71.10	8.28	2.31	61.98	5.02	1.54
[N4111][bti]	0.36	0.48	3.38	0.19	3.32	54.10	4.43	0.63
[N7111][bti]	8.04	8.08	19.29	8.06	3.74	55.94	0.06	4.45
[N6111][bti]	4.29	4.65	8.32	4.37	0.52	55.71	2.29	2.36
[N111C2O][bti]	1.87	0.75	10.43	1.63	4.26	51.55	4.22	1.02
[N8111][bti]	8.78	8.43	30.42	8.74	4.01	57.38	0.72	3.52
[tmpa][bti]	1.65	0.64	10.03	1.45	4.28	52.48	4.60	0.85
[C23guan][bti]	24.90	16.13	14.37	23.87	12.00	68.47	5.20	3.84
[NH221][bti]	2.81	1.76	9.70	2.58	6.08	53.08	5.64	0.39
[NH114][bti]	1.07	0.18	12.57	0.88	4.65	54.10	4.94	0.09
[NH11(i-3)][bti]	2.12	1.07	10.47	1.89	5.42	52.75	4.97	0.31
[DEME][bti]	1.23	1.78	5.31	1.36	2.13	56.01	4.43	0.04
[N222(2O1)][bti]	1.89	2.15	3.64	1.95	1.86	57.19	4.92	0.69
[N222(1O1)][bti]	0.40	0.14	3.65	0.29	3.71	56.43	5.90	1.49
[NH222][bti]	1.11	2.02	15.06	1.31	2.55	53.09	2.84	2.29
[N222(12)][bti]	16.21	11.85	4129.83	15.59	7.26	64.80	4.19	1.45
[N2225][bti]	3.64	3.31	12.06	3.58	0.90	59.12	5.33	1.20
[C27guan][Cl]	25.24	17.90	162.00	24.04	16.93	65.69	1.58	1.40
[C35guan][Cl]	2.36	1.44	45.75	2.41	5.17	66.91	9.13	8.35
[C23guan][Cl]	28.36	19.56	31.48	26.69	16.53	64.66	0.95	3.63
[MTEOA][MSO4]	46.04	22.30	114.02	40.68	5.25	64.14	6.14	1.53
[C27guan][BF4]	11.02	8.59	17.53	10.57	10.92	64.39	4.22	0.80
[C15guan][BF4]	20.09	11.09	36.32	17.40	6.24	62.66	7.11	1.12
[C23guan][BF4]	20.28	14.25	30.40	18.96	13.81	64.39	2.88	1.91
[DEME][BF4]	3.17	5.70	35.17	4.98	10.72	48.15	15.21	0.25
[N8444][TfO]	26.41	19.64	53.62	25.18	15.17	63.12	0.78	5.37
[bhoedma][Br]	28.22	23.73	10.12	26.52	15.54	47.18	8.73	21.08
[ehoedma][Br]	27.33	24.23	19.37	25.85	16.15	41.25	11.24	25.21
[hhoedma][Br]	30.33	24.21	5.11	28.39	16.01	51.66	7.13	18.12
[hoedmpa][Br]	27.56	23.80	14.32	25.98	15.67	44.44	9.83	22.96
[OHea][f]	16.49	12.48	104.96	14.80	2.67	44.68	0.79	14.80

Table 4.4: Deviations of experimental data and calculated density of pyridinium based ionic liquids

Abbreviation	YG	RR	Bhirud	HT	VSY	VSD	MH	VZ
[4MOPY][BEI]	10.84	9.69	35.12	10.79	6.66	60.84	1.69	0.71
[bmpy][bti]	0.83	1.81	111.15	1.13	2.21	55.34	3.44	0.25
[N-epy][bti]	4.68	3.24	42.97	4.26	6.71	52.19	5.44	1.22
[pmpy][bti]	0.51	0.66	187.26	0.17	3.25	54.25	3.67	0.19

[N-bupy][bti]	1.67	0.42	155.21	1.31	4.16	54.18	4.30	0.42
[mbpyr][bti]	5.46	6.49	120.85	5.78	2.28	53.29	1.00	4.85
[bpyr][bti]	4.95	3.74	143.27	4.60	7.35	55.71	7.49	3.74
[4MOPY][bti]	9.10	8.83	61.12	9.19	4.28	58.47	0.69	2.38
[4MOPY][dca]	20.09	12.75	143.36	18.77	6.19	63.42	5.94	1.17
[py][EOESO4]	1.30	0.31	65.55	1.08	5.35	51.16	4.60	3.05
[N-bupy][PF6]	7.92	6.10	40.73	6.85	2.75	50.72	3.69	7.71
[N-epy][BF4]	6.79	7.95	26.84	7.88	12.34	47.77	15.35	0.91
[bpyr][BF4]	0.95	3.14	28.89	2.31	8.00	51.52	12.56	0.50
[4MOPY][BF4]	15.76	9.49	29.93	13.62	3.98	58.69	6.09	3.73
[N-epy][ta]	0.95	0.62	23.91	0.50	2.59	50.03	6.36	4.95
[mbpyr][TfO]	10.24	10.69	14.12	10.27	6.22	49.56	3.92	11.79
[4MOPY][TfO]	8.75	7.71	22.86	8.52	3.10	57.74	2.57	3.47
[mbupy][BF4]	3.14	0.00	28.87	1.56	5.17	53.78	11.01	1.17
[N-bupy][BF4]	1.81	3.79	32.41	3.20	8.72	49.41	12.78	1.10

4.2 Discussion

The result of the comparative study is as shown in the previous sub-chapter. It is mentioned earlier that the comparative study is carried out within 8 correlations, by which 7 are the one used for calculating the density of normal liquids, whilst the other one is a generalized model for estimating the density of ionic liquids.

The normal liquid correlations were selected because the main objective of this project is to determine the accuracy of normal liquids correlations to be applied to ionic liquids as to check the feasibility of the correlations. This is because, if the accuracy is known, the correlation that yields low percent deviation can be considered as one of the alternative to estimate the density of ionic liquids.

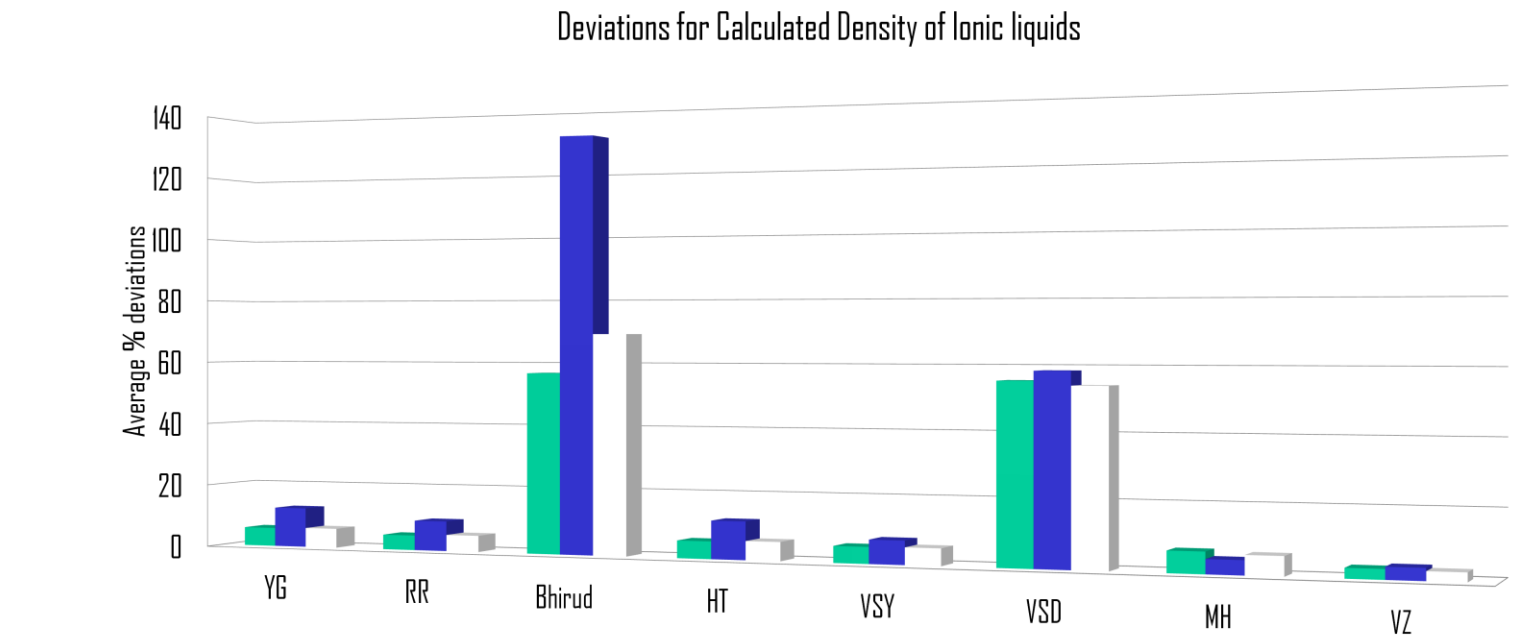
From the data above, the generalized model by Valderrama and Zarricueta yields the lowest percentage of deviations, with the average of 3.23%. Meanwhile, the highest percentage of deviation is produced by Bhirud's model with the average of 77.48%. The minimum and maximum deviations are also shown in Table 4.1.

According to the presented data, it can be observed that from the deviations, the models by BH and VSY show high values of average absolute percent deviations. This represents a large amount of error estimating the density using the two models. The maximum deviation calculated from each ionic liquid is obtained from the Bhirud's model with the value of 4129.8% which is resulted from triethyldodecylammonium bis[(trifluoromethyl)sulfonyl]imide, [N222(12)][bti].

The data obviously shows that Bhirud's is not applicable for the estimation of certain ammonium-based ionic liquid. However, it would not be fair to conclude that Bhirud is not a good model, as for 1-ethyl-3-methylidimazolium thiocyanate, the deviation obtained from Bhirud's results in only 0.48% which is the lowest deviation compared to other correlations for that ionic liquid.

There are quite a number of acceptable minimum deviations that is successfully obtained from this study. Yamada and Gunn's, Reid's, Hankinson and Thomson's, Mchaweh's and Valderrama and Zarricueta's models, all yield a deviation of less than 0.1% and even 0% error for certain ionic liquids. For example, Reid's had resulted in 0% of deviation for 4-methyl-n-butylpyridinium tetrafluoroborate and Valderrama and Zarricueta's had yield a 0% deviation for 1,3-dimethylidimazolium methoxyethyl sulfate. Other data can be referred to Table 4.2, Table 4.3 and Table 4.4.

The following Figure 4.1 shows the comparison of the average deviations calculated from different correlations. From the figure, the difference in the percentage can be simply explained illustratively.



	YG	RR	Bhirud	HT	VSY	VSD	MH	VZ
Imidazolium	5.81	4.65	56.82	5.46	5.15	55.43	6.58	3.09
Ammonium	12.45	9.41	131.22	11.86	7.36	58.42	4.43	3.73
Pyridinium	6.09	5.13	69.18	5.88	5.33	54.11	5.93	2.81

Figure 4.1: Comparison of Deviations for Calculated Density of Ionic Liquids

From Figure 4.1, it is shown that the lowest average percent deviation is presented by Valderrama and Zarricueta with the average percentage of 3.23%, and the highest would be Bhirud's which shows a very high average deviation in estimating the ammonium-based ionic liquids – 77.48%, followed by Valderrama and Abu Sharkh's (VSD) with the second highest total average of 56.10%. Other correlations result in less than 10% of average absolute percent deviation which is 7.58% for Yamada and Gunn's, 7.18% by Hankinson and Thomson's, 5.96% for Mchaweh's, 5.94% by Reid's, 5.75% by Valderrama and Abu Sharkh's (VSY).

CHAPTER 5
CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Through this study, it is found that the model that gives out the lowest average percent deviation is Valderrama and Zarricueta. The model that gives the highest average percent deviation is Bhirud and Valderrama and Abu Sharkh (VSD). However, from the presented data, Bhirud's and VSD's do not shows a constant high deviation, which in fact, Bhirud's do successfully yield the lowest percentage of deviations compared to other correlations for certain ionic liquids, where in this case, 1-ethyl-3-methylidimazolium thiocyanate with the deviation of 0.48%. Therefore, through this study, it can be concluded that the correlations presented is the best correlation for certain ionic liquids, even if not for all.

In this work, it is observed that the deviations yielded from Valderrama and Zarricueta's are mostly below 20%. Therefore, in overall, it is conclude that the most appropriate correlation for estimating the density of ionic liquids would be the model developed by Valderrama and Zarricueta, wherein it can be confidently used for any ionic liquids.

This study had successfully determined the accuracy of the selected correlations for estimating the density of 214 ionic liquids. From the study, the objective of the project work is finally achieved.

5.2 Recommendation

For both the project and institutional aspects, there are 2 things where I would like to voice out my opinions:

- The student should be exposed to various sources and wide access to the educational search engine (e.g ScienceDirect). This is because; there are too many useful documents that have limited access, which cause the student not to be able to get useful information for the project works.
- The time constraints due to the tri-semester system had gives a very limited duration for both students and lecturers. Wider view of the project studied can be explored by the students if the time given is longer, herein referred to the previous two-semester system.

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APPENDIX

APPENDIX 1 - Density data of imidazolium-based ionic liquids

IUPAC	Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)
1-methylidimazolium chloride	[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832
1-ethyl-3-methylimidazolium(2,2,2-trifluoro-n-(trifluoromethyl sulfonyl))acetamide	[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600
1-butyl-3-methylimidazolium 1,1,2,2-tetrafluoroethane sulfonate	[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240
1-dodecyl-3-methylimidazolium 1,1,2,2-tetrafluoroethane sulfonate	[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360
1-ethyl-3-methylimidazolium 1,1,2,2-tetrafluoroethane sulfonate	[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020
1-heptyl-3-methylimidazolium 1,1,2,2-tetrafluoroethane sulfonate	[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740
1-butyl-3-methylimidazolium 1,1,2,3,3,3-hexafluoropropane sulfonate	[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090
1-butyl-3-methylimidazolium 1,1,2-trifluoro-2-(perfluoroethoxy)ethane sulfonate	[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230
1-butyl-3-methylimidazolium 1,1,2-trifluoro-2-(trifluoromethoxy)ethane sulfonate	[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930
1-butyl-3-methylimidazolium 2-(1,2,2,2-tetrafluoroethoxy)-1,1,2,2-tetrafluoroethane sulfonate	[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490
1-butyl-3-methylimidazolium acetate	[bmim][Ac]	198	624.6	847.3	24.5	658.2	0.6681	298.15	1.0550
1-ethyl-3-methylimidazolium acetate	[emim][Ac]	170	578.8	807.1	29.2	544.0	0.5889	298.15	1.0270
1-ethyl-3-methylimidazolium bis(pentafluoroethylsulfonyl)imide	[emim][BEI]	491	853.1	1231.4	21.9	1045.4	0.2895	298.15	1.5900
1-butyl-3-methylimidazolium bis(pentafluoroethylsulfonyl)imide	[bmim][BEI]	505	841.3	1175.4	19.3	1117.4	0.3837	298.10	1.5140
1,2-dimethyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dmprim][bti]	419	867.4	1269.7	27.5	988.6	0.3226	295.15	1.4567
1,2-dimethyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dmprim][bti]	419	867.4	1269.7	27.5	988.6	0.3226	299.15	1.4810
1,3-dibutylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dbim][bti]	461	931.1	1305.0	22.3	1161.5	0.4349	298.15	1.4910
1,3-diethyl-4-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[E1,3M4I][bti]	419	867.4	1269.7	27.5	988.6	0.3226	295.15	1.4320
1,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dmim][bti]	377	783.2	1235.7	35.8	835.8	0.1418	295.15	1.5590
1-decyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[decmim][bti]	504	999.7	1345.1	18.7	1332.8	0.5741	298.15	1.2710
1-heptyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[hpmim][bti]	461	931.1	1305.0	22.3	1161.5	0.4349	298.15	1.3440
1-nonyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[nmim][bti]	490	976.8	1331.2	19.8	1275.7	0.5276	298.15	1.2990
1-pentyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[pmim][bti]	433	885.3	1281.1	25.6	1047.2	0.3442	298.15	1.4030
1-propyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[prmim][bti]	405	839.6	1259.3	29.9	933.0	0.2573	298.15	1.4750
1,2-dimethyl-3-ethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dmeim][bti]	392	817.8	1235.8	31.6	888.9	0.2492	293.15	1.5100
1,2-dimethyl-3-ethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dmeim][bti]	405	833.9	1254.1	29.7	948.4	0.2447	298.15	1.4802
ethoxymethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[eomim][bti]	421	862.0	1285.2	29.0	948.6	0.2694	298.15	1.4960
1-(1-phenylalkyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[Ph(CH2)mim][bti]	453	948.1	1429.7	28.1	1039.5	0.2139	298.15	1.4910

1-(2-phenylalkyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[Ph(CH2)2mim][bti]	467	971.0	1436.9	26.1	1096.6	0.2573	298.15	1.4700
1-(3-phenylalkyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[Ph(CH2)3mim][bti]	481	993.8	1444.9	24.3	1153.7	0.3018	298.15	1.4550
1-butyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[bdmim][bti]	433	890.3	1281.1	25.5	1045.7	0.3669	298.15	1.4200
1-dodecyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[C12mim][bti]	532	1045.5	1374.6	16.8	1447.0	0.6662	293.15	1.2460
1-methyl-3-ethyl-4-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[memim][bti]	392	817.8	1235.8	31.6	888.9	0.2492	293.15	1.4700
1-methyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[mmim][bti]	377	793.8	1239.9	35.8	818.8	0.1752	295.15	1.5590
1-propyl-2,3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[pdmim][bti]	419	867.4	1269.7	27.5	988.6	0.3226	295.15	1.4567
1-trifluoroethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[C2F3mim][bti]	431	788.8	1202.7	29.2	871.5	0.1879	293.15	1.6600
1-butyl-3-methylidimazolium bromide	[bmim][Br]	219	586.8	834.9	29.8	583.3	0.4891	298.40	1.2990
1-[2-(2-methoxyethoxy)ethyl]-3-methylidimazolium chloride	[moeemim][Cl]	221	625.8	863.6	24.8	657.1	0.5707	298.15	1.1400
1-butyl-3-methylidimazolium chloride	[bmim][Cl]	175	558.0	789.0	27.8	568.8	0.4908	298.15	1.0800
1-hexyl-3-methylidimazolium chloride	[hmim][Cl]	203	603.8	829.2	23.5	683.0	0.5725	298.15	1.0300
1-octyl-3-methylidimazolium chloride	[omim][Cl]	231	649.6	869.4	20.3	797.2	0.6566	298.10	1.0000
1-benzyl-3-methylidimazolium chloride	[Bemim][Cl]	209	653.4	921.3	28.4	631.8	0.5145	298.15	1.1930
1-dodecyl-3-methylidimazolium chloride	[C12mim][Cl]	287	741.1	951.5	16.0	1025.6	0.8212	298.15	0.8806
1-ethyl-3-methylidimazolium chloride	[emim][Cl]	147	512.3	748.6	34.2	454.5	0.4165	294.65	1.1860
1-methyl-3-methylidimazolium chloride	[mmim][Cl]	133	489.4	728.2	38.5	397.4	0.3825	298.15	1.1399
1-p-chlorobenzyl-3-methylidimazolium chloride	[ClBenmim][Cl]	243	695.8	969.6	26.8	682.6	0.5521	298.15	1.2670
1-p-fluorobenzyl-3-methylidimazolium chloride	[FBenMim][Cl]	227	657.6	913.1	26.4	652.0	0.5660	298.15	1.2830
1,3-dibutylimidazolium chloride	[dbim][Cl]	217	626.7	849.2	21.8	740.1	0.6144	298.15	1.0082
1-butyl-3-methylidimazolium dicyanamide	[bmim][dca]	205	783.0	1035.8	24.4	712.0	0.8419	297.15	1.0580
1-ethyl-3-methylidimazolium dicyanamide	[emim][dca]	177	737.2	999.0	29.1	597.8	0.7661	298.15	1.0600
1-octyl-3-methylidimazolium dicyanamide	[omim][dca]	261	863.9	1103.9	18.4	957.4	0.9543	298.15	1.0000
1-ethyl-3-methylidimazolium dicyanoamides	[emim][dca]	177	737.2	999.0	29.1	597.8	0.7661	298.15	1.0600
1-ethyl-3-methylidimazolium diethyleneglycol monomethylethersulfate	[emim][DEGlyMSO4]	310	826.2	1162.9	28.1	862.3	0.5176	298.15	1.2365
1,3-dimethylidimazolium dimethyl phosphate	[dmim][DMPO4]	222	623.0	880.4	28.6	598.4	0.5065	303.15	1.2530
1-ethyl-2,3-dimethylidimazolium ethyl sulfate	[edmim][ESO4]	250	740.5	1082.6	35.8	715.3	0.4341	353.15	1.1970
1-ethyl-3-methylidimazolium ethyl sulfate	[emim][ESO4]	236	712.7	1067.5	40.5	659.8	0.3744	298.15	1.2388
1-octyl-3-methylidimazolium hexafluorophosphate	[moim][PF6]	340	635.5	800.1	14.0	1007.9	0.9069	298.15	1.2360
1-[2-(2-methoxyethoxy)ethyl]-3-methylidimazolium hexafluorophosphate	[moeemim][PF6]	330	622.3	795.3	16.1	850.8	0.8676	298.15	1.3200
1-butyl-2,3-dimethylidimazolium hexafluorophosphate	[bdmim][PF6]	298	582.4	746.3	16.2	818.0	0.8526	295.65	1.2416

1-heptyl-3-methylidimazolium hexafluorophosphate	[hpmim][PF6]	326	623.2	787.8	14.7	933.8	0.9055	298.15	1.2620
1-nonyl-3-methylidimazolium hexafluorophosphate	[nmim][PF6]	354	669.0	834.1	13.4	1048.1	0.9680	298.15	1.2120
1-octyl-3-propylimidazolium hexafluorophosphate	[oprim][PF6]	368	691.9	857.6	12.8	1105.2	0.9937	298.15	1.1182
1-pentyl-3-methylidimazolium hexafluorophosphate	[pmim][PF6]	298	577.5	742.1	16.3	819.6	0.8316	294.10	1.3330
ethoxymethyl-3-methylidimazolium hexafluorophosphate	[eommim][PF6]	286	554.1	723.7	18.2	721.0	0.7692	298.15	1.4000
methyloxymethyl-3-methylidimazolium hexafluorophosphate	[mommim][PF6]	272	531.2	701.2	19.3	663.9	0.7274	298.15	1.4800
1-(3-phenylalkyl)-3-methylidimazolium hexafluorophosphate	[Ph(CH2)3mim][PF6]	346	686.0	883.8	16.3	926.1	0.8053	298.15	1.4070
1-propyl-3-methylidimazolium hexafluorophosphate	[prmim][PF6]	270	531.7	696.7	18.3	705.4	0.7504	293.00	1.3330
1-hexyl-3-ethylimidazolium hexafluorophosphate	[C2C6I][PF6]	326	623.2	787.8	14.7	933.8	0.9055	298.15	1.2622
1-octyl-3-ethylimidazolium hexafluorophosphate	[C2C8I][PF6]	354	669.0	834.1	13.4	1048.1	0.9680	298.15	1.2118
1-butyl-3-methylidimazolium hydrogen sulfate	[bmim][HSO4]	235	782.4	1103.8	43.2	664.9	0.7017	298.15	1.2770
1-ethyl-3-methylidimazolium hydrogen sulfate	[emim][HSO4]	207	736.7	1073.8	57.4	550.7	0.6394	298.15	1.3673
1-methylidimazolium hydrogen sulfate	[mim][HSO4]	179	685.5	1019.6	91.7	412.2	0.7158	298.15	1.4835
1-butyl-3-methylidimazolium iodide	[bmim][I]	266	613.7	871.2	28.6	607.5	0.4831	298.15	1.4400
1-butyl-3-methylidimazolium methane sulfonate	[bmim][mesy]	234	713.1	1054.8	37.4	701.3	0.3990	373.15	1.1284
1-ethyl-3-methylidimazolium methane sulfonate	[emim][mesy]	206	667.4	1026.0	48.1	587.1	0.3307	298.15	1.2437
1,3-dimethylidimazolium methoxyethyl sulfate	[dmim][MOESO4]	252	735.1	1094.4	38.9	675.4	0.3854	298.15	1.3140
1,3-dimethylidimazolium methyl sulfate	[dmim][MSO4]	208	666.9	1040.0	52.9	545.6	0.3086	298.15	1.3280
1-butyl-3-methylidimazolium methyl sulfate	[bmim][MSO4]	250	735.6	1081.6	36.1	716.9	0.4111	298.15	1.2124
1-butyl-3-methylidimazolium nonafluorobutane sulfonate	[bmim][NfO]	438	762.3	1028.8	17.3	1004.8	0.5150	295.15	1.4730
1-octyl-3-methylidimazolium nonafluorobutane sulfonate	[omim][NfO]	494	843.2	1094.2	14.2	1250.2	0.6591	298.15	1.3300
1-butyl-3-methylidimazolium octyl sulfate	[bmim][C8S]	349	895.7	1189.8	20.2	1116.7	0.7042	298.15	0.9971
1-[2-(2-methoxyethoxy)ethyl]-3-methylidimazolium tetrafluoroborate	[moeoemim][BF4]	272	562.9	720.2	18.8	743.3	0.9644	298.15	1.2200
1-butyl-2,3-dimethylidimazolium tetrafluoroborate	[bdmim][BF4]	240	523.1	671.0	18.9	710.5	0.9476	300.15	1.0935
1-decyl-3-methylidimazolium tetrafluoroborate	[dmim][BF4]	310	632.5	784.6	14.5	997.7	1.0817	298.15	1.0400
1-propyl-3-methylidimazolium tetrafluoroborate	[prmim][BF4]	212	472.3	619.7	21.8	597.9	0.8479	298.15	1.2400
ethyloxymethyl-3-methylidimazolium tetrafluoroborate	[moemim][BF4]	228	494.8	647.0	21.7	613.5	0.8686	298.15	1.2600
methyloxymethyl-3-methylidimazolium tetrafluoroborate	[mommim][BF4]	214	471.9	623.7	23.3	556.4	0.8291	298.15	1.3300
1-butyl-3-methylidimazolium thiocyanate	[bmim][tca]	197	763.1	1047.4	19.4	780.7	0.4781	298.15	1.0696
1-ethyl-3-methylidimazolium thiocyanate	[emim][SCN]	169	717.3	1013.6	22.3	666.4	0.3931	298.15	1.1140
1-ethyl-3-methylidimazolium trifluoroacetate	[emim][ta]	224	562.8	775.7	24.2	610.4	0.5664	298.15	1.3900
1-(4-methoxyphenyl)-3-methylidimazolium trifluoromethane sulfonate	[mpmi][TfO]	338	830.4	1184.7	28.0	827.7	0.4481	323.15	1.3200

1,3-dibutylimidazolium trifluoromethane sulfonate	[dbim][TfO]	330	776.4	1072.0	23.2	922.0	0.5325	303.15	1.3000
1-benzyl-3-methylidimazolium trifluoromethane sulfonate	[Bemim][TfO]	322	803.0	1158.0	29.0	813.7	0.4118	303.15	1.3000
1-octyl-3-methylidimazolium trifluoromethane sulfonate	[omim][TfO]	344	799.2	1088.7	21.6	979.1	0.5766	298.15	1.1200
1,2-dimethyl-3-propylimidazolium tris(trifluoromethylsulfonyl)methide	[dmpim][TMEM]	550	1039.3	1568.6	23.9	1212.0	0.1526	298.15	1.5970
1-butyl-3-methylimidazolium tris(trifluoromethylsulfonyl)methide	[bmim][TMEM]	550	1034.4	1571.4	24.0	1213.6	0.1320	297.65	1.5630
1-butyl-3-methylimidazolium tetrafluoroborate	[bmim][BF4]	226	484.6	632.3	20.4	672.0	0.8489	298.15	1.2080
1-ethyl-3-methylimidazolium tetrafluoroborate	[emim][BF4]	198	438.9	585.3	23.6	557.8	0.7685	295.15	1.2400
1-hexyl-3-methylimidazolium tetrafluoroborate	[hmim][BF4]	254	530.4	679.1	17.9	786.2	0.9258	298.15	1.1484
1-n-octyl-3-methylimidazolium tetrafluoroborate	[omim][BF4]	282	576.1	726.1	16.0	900.4	0.9954	313.15	1.0800
1-butyl-3-ethylimidazolium bis(trifluoromethylsulfonyl)imide	[beim][bti]	433	874.7	1275.9	25.6	1064.2	0.3093	295.15	1.4040
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[bmim][bti]	419	851.8	1265.0	27.6	1007.1	0.2656	295.15	1.4290
1,3-diethylimidazolium bis(trifluoromethylsulfonyl)imide	[deim][bti]	405	829.0	1254.7	29.9	950.0	0.2231	295.15	1.4520
dimethyl-3-ethylimidazolium bis(trifluoromethylsulfonyl)imide	[dmeim][bti]	405	833.9	1254.1	29.7	948.4	0.2447	298.15	1.4802
1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	[dmim][bti]	377	783.2	1235.7	35.8	835.8	0.1418	298.15	1.5590
1-ethyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	[edmim][bti]	405	833.9	1254.1	29.7	948.4	0.2447	295.15	1.4950
1-ethyl-3,5-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	[eDmim][bti]	405	833.9	1254.1	29.7	948.4	0.2447	295.15	1.4700
1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[emim][bti]	391	806.1	1244.9	32.6	892.9	0.1818	295.15	1.5200
1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[hmim][bti]	447	897.6	1287.3	23.9	1121.3	0.3539	313.15	1.3560
1-isobutyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[ibmim][bti]	419	851.4	1270.4	27.8	1005.4	0.2501	295.15	1.4280
5-methyl-1,3-diethylimidazolium bis(trifluoromethylsulfonyl)imide	[mdeim][bti]	419	856.8	1264.7	27.4	1005.5	0.2875	295.15	1.4320
1-methyl-3-ethylimidazolium bis(trifluoromethylsulfonyl)imide	[meim][bti]	391	806.1	1244.9	32.6	892.9	0.1818	298.15	1.5252
1-metoxyethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[moemim][bti]	405	851.4	1280.6	27.9	965.6	0.2208	295.15	1.4960
1-octyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[omim][bti]	475	943.4	1311.9	21.0	1235.6	0.4453	313.15	1.3110
1-trifluoroethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[tfemim][bti]	445	800.7	1205.3	26.6	942.3	0.2004	295.15	1.6560
1-octyl-3-methylimidazolium chloride	[omim][Cl]	231	638.9	860.1	20.3	814.2	0.6190	298.15	1.0070
1-ethyl-3-methylimidazolium ethyl sulfate	[emim][EtSO4]	236	702.1	1061.1	40.4	676.8	0.3368	313.15	1.2250
1-butyl-3-methylimidazolium heptafluorobutanoate	[bmim][hb]	352	644.9	836.7	15.6	894.0	0.7249	295.15	1.1330
1-ethyl-3-methylimidazolium heptafluorobutanoate	[emim][hb	324	599.2	793.9	17.4	779.8	0.6393	295.15	1.4500
1-butyl-3-ethylimidazolium methylsulfonate	[beim][MsO]	248	725.4	1062.7	33.5	775.4	0.3986	298.15	1.1400
1-ethyl-3-methylimidazolium methylsulfonate	[emim][MsO]	206	656.8	1019.5	48.0	604.0	0.2930	298.15	1.2400
1-butyl-3-ethylimidazolium nonafluorobutanesulfonate	[beim][NfO]	452	774.6	1038.5	16.4	1078.9	0.5256	295.15	1.4270
1-butyl-3-methylimidazolium nonafluorobutanesulfonate	[emim][NfO]	438	752.4	1012.1	16.7	1031.5	0.5159	295.15	1.4430
1-n-butyl-3-methylimidazolium nitrate	[bmim][NO3]	201	684.3	946.3	27.3	662.9	0.6039	313.15	1.1490

1-n-butyl-3-methylimidazolium hexafluorophosphate	[bmim][PF6]	284	544.0	708.9	17.3	779.5	0.7553	313.15	1.3460
1-ethyl-3-methylimidazolium hexafluorophosphate	[emim][PF6]	256	498.2	663.5	19.5	665.3	0.6708	298.15	1.4133
1-hexyl-3-methylimidazolium hexafluorophosphate	[hmim][PF6]	312	589.7	754.3	15.5	893.7	0.8352	298.15	1.2781
1-n-octyl-3-methylimidazolium hexafluorophosphate	[omim][PF6]	340	635.5	800.1	14.0	1007.9	0.9069	313.15	1.2110
1-butyl-3-ethylimidazolium trifluoroacetate	[beim][ta]	266	631.4	838.0	19.6	781.7	0.6936	295.15	1.1830
1-butyl-3-methylimidazolium trifluoroacetate	[bmim][ta]	252	608.6	817.2	20.9	724.6	0.6509	295.15	1.2090
1,3-diethylimidazolium trifluoroacetate	[deim][ta]	238	585.7	796.5	22.4	667.5	0.6085	295.15	1.2500
1-ethyl-3-methylimidazolium trifluoroacetate	[emim][ta]	224	562.8	775.7	24.2	610.4	0.5664	295.15	1.2850
1-butyl-3-ethylimidazolium trifluoromethanesulfonate	[beim][TfO]	302	720.0	1032.1	27.0	824.8	0.4091	295.15	1.2700
1-butyl-3-methylimidazolium trifluoromethanesulfonate	[bmim][TfO]	288	697.1	1016.3	29.4	767.6	0.3677	298.15	1.2980
1,3-diethylimidazolium trifluoromethanesulfonate	[deim][TfO]	274	674.2	1000.7	32.3	710.5	0.3276	295.15	1.3300
1-dodecyl-3-ethylimidazolium trifluoromethanesulfonate	[doeim][TfO]	413	903.0	1168.6	16.0	1281.6	0.7552	295.15	1.1000
1-ethyl-3,5-dimethylimidazolium trifluoromethanesulfonate	[edmim][TfO]	274	679.2	1001.9	32.0	709.0	0.3499	295.15	1.3340
1-ethyl-3-methylimidazolium trifluoromethanesulfonate	[emim][TfO]	260	651.4	985.2	35.8	653.4	0.2891	298.15	1.3900

APPENDIX 2 - Density data of ammonium-based ionic liquids

IUPAC	Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)
tetraethylammonium (2,2,2-trifluoro-n-(trifluoromethyl sulfonyl) acetamide	[TEA][tsac]	374	686.1	913.2	19.1	970.2	0.6591	298.15	1.3700
trimethylalylammonium (2,2,2-trifluoro-n-(trifluoromethyl sulfonyl) acetamide	[TMAlA][tsac]	344	637.0	875.2	22.5	842.3	0.5475	298.15	1.3800
trimethylethylammonium (2,2,2-trifluoro-n-(trifluoromethyl sulfonyl)acetamide	[TMEA][tsac]	332	617.4	854.1	23.3	798.8	0.5257	298.15	1.4000
trimethylisopropylammonium (2,2,2-trifluoro-n-(trifluoromethyl sulfonyl) acetamide	[TMiPA][tsac]	346	639.9	876.1	21.9	854.2	0.5536	298.15	1.4100
trimethylpropylammonium (2,2,2-trifluoro-n-(trifluoromethyl sulfonyl) acetamide	[TMPA][tsac]	346	640.3	873.7	21.7	855.9	0.5700	298.15	1.3800
diethyl methyl (quarternary) ammonium bis(pentafluoroethylsulfonyl) imide	[NH221][BEI]	468	743.8	1056.3	21.5	1053.3	0.3534	298.15	1.5100
dimethyl isopropyl (quarternary) ammonium bis(pentafluoroethylsulfonyl) imide	[NH11(i-3)][BEI]	468	743.8	1056.3	21.5	1053.3	0.3534	298.15	1.5300
[bis(bishexylamino)methylene]dimethylammonium bis[(trifluoromethyl)sulfonyl]imide	[C27guan][bti]	705	1262.0	1529.0	9.8	2167.1	1.0120	298.15	1.2000
[bis(butylethylamino)methylene]dimethylammonium bis[(trifluoromethyl)sulfonyl]imide	[C15guan][bti]	537	987.5	1271.0	15.6	1481.8	0.7803	298.15	1.3600
di(iso)propylethylheptylammonium bis[(trifluoromethyl)sulfonyl]imide	[N723'3'][bti]	509	897.6	1176.6	16.1	1408.9	0.6653	293.15	1.2700
dimethylethylbutylammonium bis[(trifluoromethyl)sulfonyl]imide	[BNM2E][bti]	410	738.3	1054.3	24.1	1012.6	0.3777	293.15	1.3700
dimethylethylpropylammonium bis[(trifluoromethyl)sulfonyl]imide	[N1123][bti]	396	715.4	1038.7	25.9	955.5	0.3334	293.15	1.4100
dimethylpropylbutylammonium bis[(trifluoromethyl)sulfonyl]imide	[N1134][bti]	424	761.2	1070.1	22.5	1069.7	0.4228	293.15	1.3400
tetradecylammonium bis[(trifluoromethyl)sulfonyl]imide	[tda][bti]	859	1470.5	1831.8	7.0	2840.1	0.4734	298.15	1.0400
tetraheptylammonium bis[(trifluoromethyl)sulfonyl]imide	[thpa][bti]	691	1195.9	1449.6	9.7	2154.8	0.9913	298.15	1.1000
tetrahexylammonium bis[(trifluoromethyl)sulfonyl]imide	[tha][bti]	635	1104.4	1353.0	11.0	1926.4	0.9857	298.15	1.1100
tetramylammonium bis[(trifluoromethyl)sulfonyl]imide	[tpa][bti]	579	1012.9	1267.0	12.8	1697.9	0.8923	298.15	1.1600
tetraoctylammonium bis[(trifluoromethyl)sulfonyl]imide	[toa][bti]	747	1287.4	1559.2	8.6	2383.2	0.8960	298.15	1.0600
tributylheptylammonium bis[(trifluoromethyl)sulfonyl]imide	[N7444][bti]	565	990.0	1247.0	13.3	1640.8	0.8585	293.15	1.1700
tributylhexylammonium bis[(trifluoromethyl)sulfonyl]imide	[N6444][bti]	551	967.1	1227.4	13.9	1583.7	0.8216	293.15	1.1500
tributylmethylammonium bis[(trifluoromethyl)sulfonyl]imide	[N1444][bti]	481	852.7	1136.3	17.7	1298.1	0.6068	296.90	1.2660
tributyloctylammonium bis[(trifluoromethyl)sulfonyl]imide	[N8444][bti]	579	1012.9	1267.0	12.8	1697.9	0.8923	293.15	1.1200
triethylheptylammonium bis[(trifluoromethyl)sulfonyl]imide	[N7222][bti]	481	852.7	1136.3	17.7	1298.1	0.6068	293.15	1.2600
triethylhexylammonium bis[(trifluoromethyl)sulfonyl]imide	[N6222][bti]	467	829.8	1119.2	18.7	1241.0	0.5608	293.15	1.2700
triethyloctylammonium bis[(trifluoromethyl)sulfonyl]imide	[N8222][bti]	495	875.6	1153.7	16.8	1355.3	0.6522	293.15	1.2500
triethyloctylammonium bis[(trifluoromethyl)sulfonyl]imide	[N8222][bti]	495	875.6	1153.7	16.8	1355.3	0.6523	298.15	1.2800

trimethylbutylammonium bis[(trifluoromethyl)sulfonyl]imide	[N4111][bti]	396	715.4	1038.7	25.9	955.5	0.3334	293.15	1.4100
trimethylheptylammonium bis[(trifluoromethyl)sulfonyl]imide	[N7111][bti]	438	784.1	1086.1	21.1	1126.8	0.4685	293.15	1.2800
trimethylhexylammonium bis[(trifluoromethyl)sulfonyl]imide	[N6111][bti]	424	761.2	1070.1	22.5	1069.7	0.4228	293.15	1.3300
trimethylmethoxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[N111C2O][bti]	384	692.1	1035.7	29.5	856.9	0.2599	298.15	1.5100
trimethyloctylammonium bis[(trifluoromethyl)sulfonyl]imide	[N8111][bti]	452	807.0	1102.5	19.8	1183.9	0.5146	293.15	1.2700
trimethylpropylammonium bis[(trifluoromethyl)sulfonyl]imide	[tmpa][bti]	382	692.6	1023.4	28.0	898.4	0.2900	298.15	1.4400
bis-hexyl-aminomethylene dimethylammonium bis[(trifluoromethyl)sulfonyl]imide	[C23guan][bti]	649	1170.5	1432.1	11.2	1938.7	1.0159	298.15	1.2000
diethylmethyl (quaternary) ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH221][bti]	368	707.4	1061.1	31.9	883.8	0.2805	298.15	1.4300
dimethylbutyl (quaternary) ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH114][bti]	382	730.3	1075.3	29.3	940.9	0.3229	298.15	1.3900
dimethylisopropyl (quaternary) ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH11(i-3)][bti]	368	707.4	1061.1	31.9	883.8	0.2805	298.15	1.4200
N,N-diethyl-N-methyl-N-(2-methoxyethyl) ammonium bis[(trifluoromethyl)sulfonyl]imide	[DEME][bti]	426	760.7	1080.7	23.5	1028.2	0.3915	293.15	1.4200
triethyl(2-methoxyethyl)ammonium bis[(trifluoromethyl)sulfonyl]imide	[N222(2O1)][bti]	440	783.6	1096.3	22.0	1085.3	0.4370	298.15	1.4000
triethyl(methoxymethyl)ammonium bis[(trifluoromethyl)sulfonyl]imide	[N222(1O1)][bti]	426	760.7	1080.7	23.5	1028.2	0.3915	298.15	1.4400
triethyl(quaternary)ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH222][bti]	382	730.3	1075.3	29.3	940.9	0.3229	298.15	1.3600
triethyldodecylammonium bis[(trifluoromethyl)sulfonyl]imide	[N222(12)][bti]	551	967.1	1227.4	13.9	1583.7	0.8216	298.15	1.2200
triethylpentylammonium bis[(trifluoromethyl)sulfonyl]imide	[N2225][bti]	452	807.0	1102.5	19.8	1183.9	0.5146	298.15	1.3300
[bis(bis-hexyl-amino)methylene]dimethylammonium chloride	[C27guan][Cl]	460	957.6	1158.9	9.2	1745.7	0.9692	298.15	0.9000
[bis(bis-octyl-amino)methylene]dimethylammonium chloride	[C35guan][Cl]	572	1140.7	1411.1	7.4	2202.6	0.5680	298.15	0.9600
bis-hexyl-amino-methylenedimethylammonium chloride	[C23guan][Cl]	404	866.1	1052.1	10.5	1517.3	1.0428	298.15	0.9000
tris(2-hydroxyethyl)methylammonium methyl sulfate	[MTEOA][MSO4]	273	865.1	1093.4	34.9	744.3	1.5130	353.15	1.3100
[bis(bis-hexylamino)methylene]dimethylammonium tetrafluoroborate	[C27guan][BF4]	512	894.8	1100.3	8.2	1832.0	0.7076	298.15	0.9700
[bis(butyl-ethylamino)methylene]dimethylammonium tetrafluoroborate	[C15guan][BF4]	343	620.3	755.9	12.2	1146.7	1.1454	298.15	1.0500
bis-hexyl-amino-methylene dimethylammonium tetrafluoroborate	[C23guan][BF4]	455	803.3	975.1	9.2	1603.5	0.9385	298.15	0.9700
N,N-diethyl-N-methyl-N-(2-methoxyethyl)ammonium tetrafluoroborate	[DEME][BF4]	233	393.5	501.4	17.1	693.1	0.9465	293.15	1.1800
tributyloctylammonium trifluoromethane sulfonate	[N8444][TfO]	448	858.2	1066.7	12.6	1458.4	0.9461	293.15	1.0200
butyl-(2-hydroxyethyl)-dimethylammonium bromide	[bhoedma][Br]	226	554.8	732.3	25.2	626.4	0.8841	298.15	1.0670
ethyl-(2-hydroxyethyl)-dimethylammonium bromide	[ehoedma][Br]	198	509.1	687.9	30.2	512.2	0.8078	298.15	1.1018

hexyl-(2-hydroxyethyl)-dimethylammonium bromide	[hhoedma][Br]	254	600.6	776.6	21.7	740.7	0.9601	298.15	1.0412
(2-hydroxyethyl)-dimethylpropylammonium bromide	[hoedmpa][Br]	212	531.9	710.1	27.5	569.3	0.8455	298.15	1.0827
2-hydroxyethylammonium formate	[OHea][f]	107	491.2	683.2	54.0	285.2	0.8979	298.15	1.2040

APPENDIX 3 - Density data of pyridinium-based ionic liquids

IUPAC	Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)
4-methyl-n-octylpyridinium bis(pentafluoroethylsulfonyl)imide	[4MOPY][BEI]	587	979.9	1291.4	15	1436.7	0.5858	298.15	1.3900
1-butyl-3-methylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[bmpy][bti]	430	852	1240.5	25.5	1038.8	0.3160	298.15	1.4120
1-ethylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[N-epy][bti]	388	778.4	1207.9	32.7	869.0	0.1671	298.15	1.5360
3-methyl-1-propylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[pmpy][bti]	416	829.1	1228.9	27.5	981.7	0.2723	298.15	1.4440
n-butylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[N-bupy][bti]	416	824.2	1229.1	27.7	983.3	0.2505	298.15	1.4490
1-butyl-4-methylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[mbpyr][bti]	430	852	1240.5	25.5	1038.8	0.3160	298.15	1.3500
1-butylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[bpyr][bti]	416	824.2	1229.1	27.7	983.3	0.2505	298.10	1.4990
4-methyl-n-octylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[4MOPY][bti]	487	943.5	1292	19.7	1267.2	0.4983	298.15	1.2900
4-methyl-n-octylpyridinium dicyanamide	[4MOPY][dca]	272	864.1	1094.3	17.2	989.1	0.9923	298.15	0.9800
pyridinium ethoxyethyl sulfate	[py][EOESO4]	248	696.1	1065.4	41.8	658.8	0.2994	298.15	1.2810
n-butylpyridinium hexafluorophosphate	[N-bupy][PF6]	281	516.3	674.4	17.3	755.6	0.7381	298.15	1.2144
1-ethylpyridinium tetrafluoroborate	[N-epy][BF4]	195	411.2	549.9	23.5	533.9	0.7495	293.10	1.3020
1-butylpyridinium tetrafluoroborate	[bpyr][BF4]	223	456.9	597.6	20.3	648.1	0.8307	298.20	1.2144
4-methyl-n-octylpyridinium tetrafluoroborate	[4MOPY][BF4]	293	576.3	720.8	15.1	932.1	1.0289	298.15	1.0800
1-ethylpyridinium trifluoroacetate	[N-epy][ta]	221	535.1	739.9	24.2	586.5	0.5483	293.10	1.2730
1-butyl-4-methylpyridinium trifluoromethane sulfonate	[mbpyr][TfO]	299	697.3	997.8	26.9	799.3	0.4153	298.15	1.1700
4-methyl-n-octylpyridinium trifluoromethane sulfonate	[4MOPY][TfO]	355	788.8	1065.7	20.1	1027.8	0.5898	298.15	1.1700
4-methyl-n-butylpyridinium tetrafluoroborate	[mbupy][BF4]	237	484.8	625.8	18.9	703.7	0.8923	298.15	1.1842
N-butylpyridinium tetrafluoroborate	[N-bupy][BF4]	223	456.9	597.6	20.3	648.1	0.8307	313.15	1.2030

$$\rho = \rho_c(0.29056 - 0.08775\omega)^{-(1-T_r)^{2/7}}$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	ρc	Tr	ρ (calc)	|%Δρ|
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	0.37646	0.513523339	1.161549877	1.829794034
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	0.42591	0.278670904	1.522969827	4.313001875
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	0.38657	0.292527899	1.355388455	2.370729193
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	0.33704	0.25734415	1.355366547	19.3104355
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	0.40919	0.301993588	1.390920186	7.39546031
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	0.36229	0.278636195	1.335585122	4.833996979
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	0.4054	0.288877047	1.440209604	2.215018036
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	0.43045	0.280929049	1.56328234	9.858210844
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	0.41586	0.281725409	1.489921481	6.957751678
[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490	0.43045	0.280929049	1.56328234	7.886980008

$$\rho = \rho_c[1 + 0.85(1 - T_r) + (1.6916 + 0.984\omega)(1 - T_r)^{\frac{1}{3}}]$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	Tr	ρc	ρ (calc)	%Δρ
[hmim][PF6]	312	589.7	754.3	15.5	893.7	0.8352	298.15	1.2781	0.395267135	0.349334228	1.271400905	0.524144835
[omim][PF6]	340	635.5	800.1	14.0	1007.9	0.9069	313.15	1.2110	0.391388576	0.337632702	1.251644292	3.356258662
[beim][ta]	266	631.4	838.0	19.6	781.7	0.6936	295.15	1.1830	0.352207637	0.340667775	1.228050423	3.808150677
[bmim][ta]	252	608.6	817.2	20.9	724.6	0.6509	295.15	1.2090	0.361172296	0.348054099	1.236116277	2.242868238
[deim][ta]	238	585.7	796.5	22.4	667.5	0.6085	295.15	1.2500	0.370558694	0.356853933	1.248234482	0.141241406
[emim][ta]	224	562.8	775.7	24.2	610.4	0.5664	295.15	1.2850	0.380495037	0.367300131	1.264886909	1.565221094
[beim][TfO]	302	720.0	1032.1	27.0	824.8	0.4091	295.15	1.2700	0.285970352	0.366391853	1.274557628	0.358868347
[bmim][TfO]	288	697.1	1016.3	29.4	767.6	0.3677	298.15	1.2980	0.2933681	0.375455967	1.287668998	0.795916933
[deim][TfO]	274	674.2	1000.7	32.3	710.5	0.3276	295.15	1.3300	0.29494354	0.385925405	1.308979892	1.580459242
[doeim][TfO]	413	903.0	1168.6	16.0	1281.6	0.7552	295.15	1.1000	0.252567174	0.321863296	1.237525143	12.50228573
[edmim][TfO]	274	679.2	1001.9	32.0	709.0	0.3499	295.15	1.3340	0.294590278	0.38674189	1.31953556	1.084290869
[emim][TfO]	260	651.4	985.2	35.8	653.4	0.2891	298.15	1.3900	0.302628908	0.398224671	1.332113521	4.164494928

$$ln\frac{P_c}{\rho RT} = ln\,V^{(0)} + \omega\, ln\,V^{(1)}$$

$$ln\,V^{(0)} = 1.39644 - 24.076T_r + 102.615{T_r}^2 - 255.719{T_r}^3 + 355.805{T_r}^4 - 256.671{T_r}^5 + 75.1088{T_r}^6$$

$$ln\,V^{(1)} = 13.4412 - 135.7437T_r + 533.380{T_r}^2 - 1091.453{T_r}^3 + 1231.43{T_r}^4 - 728.227{T_r}^5 + 176.7377{T_r}^6$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	R	Tr	V(0)	V(1)	ln V(0) + ω ln V(1)	ρ (calc)	%Δρ
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	0.083144621	0.513523339	1.581777927	0.544275485	0.180921477	1.36987352	15.77700469
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	0.083144621	0.278670904	1.128435217	0.300384017	-0.477748679	1.639136738	12.2696396
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	0.083144621	0.292527899	1.163988841	0.37839759	-0.293527674	1.375184998	3.86593643
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	0.083144621	0.25734415	1.069147081	0.139207585	-1.523386655	2.856391044	151.4428735
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	0.083144621	0.301993588	1.187174286	0.421579282	-0.151724727	1.411618526	6.017408403
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	0.083144621	0.278636195	1.128343501	0.300164364	-0.589631193	1.490825778	17.0192918
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	0.083144621	0.288877047	1.154818298	0.359641999	-0.360528352	1.232213906	12.54691941
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	0.083144621	0.280929049	1.134372226	0.314402274	-0.508927202	1.20118067	15.58814689
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	0.083144621	0.281725409	1.136452041	0.319219504	-0.45273294	1.325857141	4.820018591
[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490	0.083144621	0.280929049	1.134372226	0.314402274	-0.508927202	1.20118067	17.10278332

$$\rho = \frac{\rho_c}{[\,V^{(0)}(1 - \omega\, V^{(1)}]}$$

$$V^{(0)} = 1 - 1.5281(1 - T_r)^{1/3} + 1.4390(1 - T_r)^{2/3} - 0.8144(1 - T_r) + 0.19045(1 - T_r)^{4/3}$$

$$V^{(1)} = \frac{(-0.296123 + 0.386914T_r - 0.0427258{T_r}^2 - 0.0480645{T_r}^3)}{(T_r - 1.00001)}$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	Tr	V(0)	V(1)	ρc	ρ (calc)	%Δρ
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	0.51352334	0.36495435	0.236819547	0.376463145	1.156538731	2.2533
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	0.2786709	0.32270363	0.267085844	0.425914817	1.522173124	4.2584
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	0.2925279	0.324805022	0.26544726	0.386566804	1.354991061	2.3407
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	0.25734415	0.319542605	0.269571655	0.337043668	1.347791927	18.6437
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	0.30199359	0.326262895	0.264317333	0.409192825	1.391886141	7.3311
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	0.2786362	0.322698414	0.267089925	0.362289832	1.332826229	4.6174
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	0.28887705	0.324247638	0.265880763	0.405435021	1.439143571	2.1394
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	0.28092905	0.323043466	0.266820079	0.430447231	1.561062357	9.7022
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	0.28172541	0.323163553	0.266726236	0.415858651	1.488757039	6.8742
[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490	0.28092905	0.323043466	0.266820079	0.430447231	1.561062357	7.7338

$$\rho = \left(0.01256 + 0.9533\frac{M}{V_c}\right)\left[\left(\frac{0.0039}{M} + \frac{0.2987}{V_c}\right){V_c}^{1.033}\right]^{\gamma(T)}$$

$$\gamma(T) = -\left[\frac{(1 - T_r)}{(1 - T_{br})}\right]^{2/7}$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	Tr	Tbr	γ	ρ (calc)	%Δρ
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	0.513523339	0.670495856	-1.117746142	1.116058984	5.67452807
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	0.278670904	0.714459295	-1.303137135	1.455210496	0.32804825
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	0.292527899	0.707811742	-1.287441749	1.300381376	1.783883963
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	0.25734415	0.779248506	-1.414289355	1.251126668	10.1343898
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	0.301993588	0.684932879	-1.255167854	1.343616001	10.54487343
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	0.278636195	0.738434493	-1.336220868	1.265273466	0.684971258
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	0.288877047	0.724348416	-1.310978251	1.389568561	1.379094309
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	0.280929049	0.742674079	-1.34125365	1.512339579	6.278255703
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	0.281725409	0.727581971	-1.319171715	1.435740335	3.068222168
[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490	0.280929049	0.742674079	-1.34125365	1.512339579	4.371261467

$$\rho = \left(\frac{MP_c}{RT_c}\right)\left[\left(0.3445\,\frac{P_c}{RT_c}\right)V_c^{\,1.0135}\right]^{-\frac{[1+(1-T_r)^{\frac{2}{7}}]}{[1+(1-T_{br})^{\frac{2}{7}}]}}$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	R	Tr = T/Tc	Tbr = Tb/Tc	$-\frac{[1+(1-T_r)^{\frac{2}{7}}]}{[1+(1-T_{br})^{\frac{2}{7}}]}$	ρ (calc)	%Δρ
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	0.083144621	0.513523339	0.670495856	-1.049613588	0.804874834	31.97474355
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	0.083144621	0.278670904	0.714459295	-1.124716119	0.644964799	55.82432882
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	0.083144621	0.292527899	0.707811742	-1.118716694	0.597842155	54.84575867
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	0.083144621	0.25734415	0.779248506	-1.16312076	0.436305362	61.59283789
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	0.083144621	0.301993588	0.684932879	-1.106722102	0.666072221	55.65431284
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	0.083144621	0.278636195	0.738434493	-1.136291918	0.521197575	59.08967228
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	0.083144621	0.288877047	0.724348416	-1.127184423	0.609558284	56.7382339
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	0.083144621	0.280929049	0.742674079	-1.137948144	0.624256349	56.13096631
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	0.083144621	0.281725409	0.727581971	-1.130275379	0.618709542	55.58438321
[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490	0.083144621	0.280929049	0.742674079	-1.137948144	0.624256349	56.91812633

$$\rho(T) = \rho_c(1 + 1.169\tau^{\frac{1}{3}} + 1.818\tau^{\frac{2}{3}} - 2.658\tau + 2.161\tau^{\frac{4}{3}})$$

$$\tau = 1 - \frac{\left(\frac{T}{T_c}\right)}{[1 + m(1 - \sqrt{T/T_c})]^2}$$

$$m = 0.480 + 1.574\omega - 0.176\omega^2$$

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	m	T/Tc	[1+m(1-(T/Tc)^1/2)]^2	τ	ρc	ρ (calc)	%Δρ
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	1.161713	0.513523	1.766833929	0.709353929	0.376463145	1.118178009	5.49543537
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	1.219784	0.278671	2.483361662	0.887784809	0.425914817	1.399976595	4.11119209
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	1.164397	0.292528	2.355068267	0.875787932	0.386566804	1.2623265	4.658119338
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	1.634953	0.257344	3.260033018	0.921060876	0.337043668	1.128028172	0.701745417
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	1.044491	0.301994	2.162375512	0.860341746	0.409192825	1.324901847	11.79082243
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	1.347804	0.278636	2.677648826	0.895939978	0.362289832	1.19614599	6.110989833
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	1.213625	0.288877	2.437766243	0.881499283	0.405435021	1.328089584	5.742400024
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	1.290803	0.280929	2.581299036	0.891167569	0.430447231	1.417487664	0.387374258
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	1.23487	0.281725	2.494593315	0.887065596	0.415858651	1.366385518	1.910587366
[bmim][FS]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490	1.290803	0.280929	2.581299036	0.891167569	0.430447231	1.417487664	2.174764368

$$\rho = \left(\frac{A}{B}\right) + \left(\frac{2}{7}\right).\left\{\frac{A.\ln B}{B}\right\}.\frac{(T - T_b)}{(T_c - T_b)}$$

$$A = a + b.\frac{M}{V_c}$$

$$B = \left(\frac{c}{V_c} + \frac{d}{M}\right).V_c^{\ \delta}$$

a = 0.3411; b = 2.0443; c = 0.5386; d = 0.0393; δ = 1.0476

Abbreviation	M	Tb (K)	Tc (K)	Pc (bar)	Vc (cm3/mol)	ω	T (K)	ρ (g/cm^3)	a	b	c	d	delta	A	B	ρ (calc)	%Δρ
[mim][Cl]	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832	0.3411	2.0443	0.5386	0.0393	1.0476	1.110703606	0.845663684	1.343378437	13.54
[emim][tsac]	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600	0.3411	2.0443	0.5386	0.0393	1.0476	1.21179766	0.86891309	1.480062256	1.37
[bmim][TFES]	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240	0.3411	2.0443	0.5386	0.0393	1.0476	1.131358517	0.881561187	1.349054416	1.89
[dmim][TFES]	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360	0.3411	2.0443	0.5386	0.0393	1.0476	1.03011837	0.921200667	1.180232211	3.89
[emim][TFES]	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020	0.3411	2.0443	0.5386	0.0393	1.0476	1.177612892	0.867668371	1.42411599	5.19
[hpmim][TFES]	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740	0.3411	2.0443	0.5386	0.0393	1.0476	1.081729103	0.898957598	1.267691367	0.50
[bmim][HFPS]	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090	0.3411	2.0443	0.5386	0.0393	1.0476	1.169930813	0.879118463	1.408189059	0.06
[bmim][TPES]	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230	0.3411	2.0443	0.5386	0.0393	1.0476	1.221063274	0.87566269	1.489366607	4.66
[bmim][TTES]	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930	0.3411	2.0443	0.5386	0.0393	1.0476	1.191239841	0.876464421	1.442946609	3.59