Experimental Densities of Binary mixture of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide or sulfolane with monoethanolamine and their molecular interaction by COSMO-RS

Mohd Azlan Kassim¹², Nor Asrina Sairi²³, Rozita Yusoff⁴⁵ and Mohamed Kheireddine Aroua¹

¹Research Centre for Carbon Dioxide Capture and Utilisation, School of Science and Technology, Sunway University, Bandar Sunway, 47500 Selangor Darul Ehsan, Malaysia.
²Chemistry Department, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia
³Universiti Malaya Center for Ionic Liquids, Chemistry Department, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia
⁴Chemical Engineering Department, Faculty of Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia
⁵Centre for Separation Science & Technology, Department of Chemical Engineering, Faculty of Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

azlanka@sunway.edu.my

Abstract. Thermophysical properties (densities, ρ) was measured for the binary mixtures of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [BMIM][NTf₂] and sulfolane with monoethanolamine (MEA) over the entire range of composition, and at different temperatures from T = (303.15 to 343.15) K. From experimental data of ρ, the excess molar volumes, Vₑ was calculated and fitted to the Redlich-Kister equation. The positive Vₑ values were observed for both of the systems indicating expansion of volume due to breakage of MEA-MEA intramolecular hydrogen bond by addition of [BMIM][NTf₂] or sulfolane. Subsequently, a quantum chemical-based COSMO-RS modelling was used to predict the molecular interaction based on non-ideal liquid phase σ-profile and σ-potential for all mixtures. It has been interpreted that weak interaction for [BMIM][NTf₂] (1) + MEA (2) and MEA (2) + sulfolane (3) system. A discussion was carried out in terms of interactions and structure factors in these binary mixtures based on results obtained.

Keyword: Redlich-Kister, excess molar volume, MEA, sulfolane, ionic liquid, COSMO-RS model.
1.0 Introduction
Non-aqueous alkanolamine solvent for CO₂ capture has been developed as an alternative solvent to the common aqueous alkanolamine solvent for CO₂ absorption process. The common aqueous alkanolamine solutions applied in the industrial CO₂ removal processes are monoethanolamine (MEA), diethanolamine (DEA), methylethanolamine (MMEA), methyldiethanolamine (MDEA), aminomethylpropanol (AMP), diethylene glycolamine (DGA,), diisopropanolamine (DIPA), piperazine (PZ), triethanoleamine (TEA) which were used either as a single or blended aqueous solution [1, 2].

Non-aqueous alkanolamine solvent has potential to substantially reduce the drawbacks posed by aqueous alkanolamine solvent such as, loss of solvent during regeneration, high energy requirement for regeneration and corrosion of equipment [3, 4] which is primarily attributed to presence of water in the mixture [5]. Hence, by replacing water with organic solvents, a considerable amount of thermal energy can be saved during the solvent heating cycle and the corrosion will also be prevented [6]. It was reported mixture of alkanolamine with using methanol, ethanol or other polar organics solvent have better solubility CO₂ solubility but was not preferable due to high vapor pressure of the polar organic solvent [7-9]. Another approach was by substituting water with polyol (glycerol, diethylene glycerol or triethylene glycol) [6, 10, 11]. However, alkanolamine - polyol mixtures tend to have high viscosity which is not preferable for process operation [12]. In this study, high boiling point solvents (1-butyl-3-methylimidazolium bis(trifluoromethylsulfonylimide) and sulfolane) were used as part of the binary mixture with MEA as a non-aqueous system due to their high thermostability and negligible vapor pressure. Ionic liquid – alkanolamine combination was reported to offers reductions in energy and also prevent corrosion of the system [13, 14], while sulfolane is one of the major components in the common industrial CO₂ absorption process called Sulfinol process [15].

The aim of this studies is to provide a wide set of precise experimental data for densities and excess molar volumes for [BMIM][NTf₂] + MEA and sulfolane + MEA systems over the 303.15–343.15 K temperature range and to discuss the data in terms of molecular interaction of the mixtures. Using the experimental density data of these mixtures, excess molar volume (\(V^E\)) is calculated. Using COSMO-RS model (COnductor-like Screening MOdel for Real Solvents) σ-profile and σ-potential for composition of mixtures is predicted. This model is independent of experimental data and uses the molecular structure to determine the Screening Charge Densities (SCDs) or the sigma profile of the pure molecule. Thermophysical data (density) is essential in the chemical industry for designing and process optimization of a chemical process for determining the mass transfer, fluid flow, heat transfer and energy consumption of the chemical process [16-18]. On the other hand, thermophysical properties data is also valuable in order to understand the intermolecular interaction with in the mixture.

2.0 Experimental Section

2.1 Material

The chemical used in this work were supplied with high purity and summarized in Table 1 with source purity and CAS number of the chemicals. The water content for 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonylimide, [BMIM][NTf₂] was 0.005 wt%, as determined by Karl Fisher titration using an 831 Karl Fischer coulometer. Fig. 1 shows the chemical structures of MEA, sulfolane and [BMIM][NTf₂]. All chemicals were used as received.

| Chemical | MEA | Sulfolane | [BMIM][NTf₂] |
|----------|-----|-----------|--------------|
| Molecular formula | \(\text{C}_2\text{H}_7\text{NO}\) | \(\text{C}_4\text{H}_8\text{O}_2\text{S}\) | \(\text{C}_{10}\text{H}_{15}\text{F}_6\text{N}_3\text{O}_4\text{S}_2\) |
2.2 Apparatus and Procedure

Density measurement of the binary mixtures was carried out using oscillating U-tube digital densitometer DDM 2910 (Rudolph Research, USA) from the temperature of 303.15 K to 363.15 K at 10 K interval with the temperature accuracy of ±0.05 K at 1 atm. The apparatus is precise within 0.0001 g cm\(^{-3}\). The calibration of the densitometer was performed using dry air and ultra-pure water (supplied) at given temperature and atmosphere pressure.

2.3 Computational Details

The structure of MEA, sulfolane and [BMIM][NTf\(_2\)] respective ions were drawn and geometry optimized using TmoleX software package. Geometry optimization was performed at Hartree-Fock theory with 6-31G* basic set. Geometry optimization calculation using Hartree-Fock level provides more meaningful accurate values while the * accounts for polarization effect of the species [19, 20]. Using the optimized geometry for each individual compounds, a single point calculation was conducted with activation of the .cosmo file generation using density functional theory (DFT) with 6-31G* basic set. Then, the .cosmo file was imported into the COSMOthermX software package (version C30_1401) with parameterization file BP_TZVP_C30_1301.ctd. [19] to obtain the σ-profile and σ-potential of the individual components and to calculate activity coefficient and Gibbs free energy of the [BMIM][NTf\(_2\)] (1) + MEA (2) and MEA (2) + sulfolane (3) binary mixtures. Within COSMOthermX software, a pseudo binary approach was adopted for the calculation of the mixture compose of the [BMIM][NTf\(_2\)] (1) +
MEA (2) whereby the cation and anion of the ionic liquid was input as separate compounds with equal mole fraction.

3.0 Result and Discussion

3.1 Pure Compounds and Their Binary Mixtures.

Verification of the equipment and procedures, the density of pure [BMIM][NTf₂], sulfolane and MEA were conducted at different temperatures and compared with readings from literatures (Table 2). The relative deviations of these results were calculated using Equation (1) and are shown in Fig. 2.

\[
\text{Relative Deviation} = \frac{Y_{\text{exp}} - Y_{\text{lit}}}{Y_{\text{exp}}}, \quad Y = \rho
\]

where \( \rho \) is the density. The subscript “exp” and “lit” denote experimental data of this work and literature values, respectively.

| \( T \)/K | \( \rho \), g cm\(^{-3} \) | [BMIM][NTf₂] | MEA | sulfolane |
|---------|----------------|---------|----|--------|
| 303.15  | 1.4135  | 1.4319  | 1.0094 | 1.2594 | 1.2604 |
| 313.15  | 1.4219  | 1.4223  | 1.0012 | 1.2517 | 1.2505 |
| 323.15  | 1.4124  | 1.4129  | 0.9931 | 1.2440 | 1.2412 |
| 333.15  | 1.4029  | 1.4035  | 0.9849 | 1.2354 | 1.2326 |
| 343.15  | 1.3935  | 1.3942  | 0.9760 | 1.2250 | 1.2224 |

1 = data from [21]
2 = data from [22]
3 = data from [23]

Fig. 2: Comparison of density for pure [BMIM][NTf₂], MEA and sulfolane with literatures; (○) [BMIM][NTf₂]Exp.; (○) [BMIM][NTf₂]Lit [21]; (▼) MEAExp.; (△) MEALit [22]; (■) sulfolaneExp.; (□) sulfolaneLit [23]
Table 3 and Table 4 summarized the experimental density values of [BMIM][NTf₂] (1) + MEA (2) and MEA (2) + sulfolane (3) mixtures. Fig. 3 illustrates the measured density of binary mixture [BMIM][NTf₂] (1) + MEA (2) throughout the entire mole fraction composition with the temperature ranging from 303.15 K to 343.15 K which shows that the density increases with the increased composition of [BMIM][NTf₂]. Similarly, Fig. 4 presents the measured density of MEA (2) + sulfolane (3) mixtures throughout the whole composition and the temperature ranging from 303.15 K to 343.15 K. In both binary mixtures, the density value decreased quasi-linear manner with the increase of temperature throughout the whole composition.

Table 3. Experimental densities (ρ), viscosity (η), excess molar volume (Vₑ), and viscosity deviation (Δη) of [BMIM][NTf₂] (1) + MEA (2) at different temperature and composition (x₁, x₂ = mole fraction) at atmospheric pressure P = 101.3 kPa.

| T = 303.15 K | x₁ | x₂ | ρ (g cm⁻³) | Vₑ (cm³ mol⁻¹) |
|--------------|----|----|------------|---------------|
| 0.0000       | 1.0000 | 1.0094 | 0.0000 |
| 0.1001       | 0.8999 | 1.1561 | 0.1000 |
| 0.2000       | 0.8000 | 1.2377 | 0.3000 |
| 0.3000       | 0.7000 | 1.2906 | 0.4500 |
| 0.4000       | 0.6000 | 1.3281 | 0.5248 |
| 0.4999       | 0.5001 | 1.3564 | 0.5111 |
| 0.6000       | 0.4000 | 1.3783 | 0.4700 |
| 0.6999       | 0.3001 | 1.3959 | 0.4000 |
| 0.8000       | 0.2000 | 1.4099 | 0.3691 |
| 0.8998       | 0.1002 | 1.4219 | 0.2792 |
| 1.0000       | 0.0000 | 1.4329 | 0.0000 |

| T = 313.15 K | x₁ | x₂ | ρ (g cm⁻³) | Vₑ (cm³ mol⁻¹) |
|--------------|----|----|------------|---------------|
| 0.0000       | 1.0000 | 1.012 | 0.0000 |
| 0.1001       | 0.8999 | 1.1475 | 0.1300 |
| 0.2000       | 0.8000 | 1.2284 | 0.4100 |
| 0.3000       | 0.7000 | 1.2805 | 0.6800 |
| 0.4000       | 0.6000 | 1.3182 | 0.7701 |
| 0.4999       | 0.5001 | 1.3464 | 0.8122 |
| 0.6000       | 0.4000 | 1.3687 | 0.7700 |
| 0.6999       | 0.3001 | 1.3861 | 0.7650 |
| 0.8000       | 0.2000 | 1.4000 | 0.7932 |
| 0.8998       | 0.1002 | 1.4123 | 0.6769 |
| 1.0000       | 0.0000 | 1.4254 | 0.0000 |

| T = 323.15 K | x₁ | x₂ | ρ (g cm⁻³) | Vₑ (cm³ mol⁻¹) |
|--------------|----|----|------------|---------------|
| 0.0000       | 1.0000 | 0.9931 | 0.0000 |
| 0.1001       | 0.8999 | 1.1382 | 0.1200 |
| 0.2000       | 0.8000 | 1.2191 | 0.3400 |
| 0.3000       | 0.7000 | 1.2714 | 0.5200 |
| 0.4000       | 0.6000 | 1.3084 | 0.6378 |
| 0.4999       | 0.5001 | 1.3366 | 0.6227 |
| 0.6000       | 0.4000 | 1.3586 | 0.5700 |
| 0.6999       | 0.3001 | 1.3761 | 0.5000 |
| 0.8000       | 0.2000 | 1.3903 | 0.4342 |
| 0.8998       | 0.1002 | 1.4027 | 0.2442 |
| 1.0000       | 0.0000 | 1.4134 | 0.0000 |
### Table 4. Experimental densities ($\rho$) and excess molar volume ($V^E$) of MEA (2) + sulfolane (3) at different temperature and composition ($x_2, x_3 =$ mole fraction) at atmospheric pressure $P = 101.3$ kPa.

| $T$ = 333.15 K | $x_2$ | $x_3$ | $\rho$ (g cm$^{-3}$) | $V^E$ (cm$^3$ mol$^{-1}$) |
|----------------|-------|-------|-----------------------|--------------------------|
| 0.0000         | 1.0000| 0.9849 | 0.0000                |                          |
| 0.1001         | 0.8999| 1.1293 | 0.1300                |                          |
| 0.2000         | 0.8000| 1.2095 | 0.3900                |                          |
| 0.3000         | 0.7000| 1.2615 | 0.5900                |                          |
| 0.4000         | 0.6000| 1.2986 | 0.6911                |                          |
| 0.4999         | 0.5001| 1.3268 | 0.6761                |                          |
| 0.6000         | 0.4000| 1.3488 | 0.6100                |                          |
| 0.6999         | 0.3001| 1.3665 | 0.5100                |                          |
| 0.8000         | 0.2000| 1.3807 | 0.4479                |                          |
| 0.8998         | 0.1002| 1.3931 | 0.2447                |                          |
| 1.0000         | 0.0000| 1.4038 | 0.0000                |                          |

| $T$ = 343.15 K | $x_2$ | $x_3$ | $\rho$ (g cm$^{-3}$) | $V^E$ (cm$^3$ mol$^{-1}$) |
|----------------|-------|-------|-----------------------|--------------------------|
| 0.0000         | 1.0000| 0.9849 | 0.0000                |                          |
| 0.1001         | 0.8999| 1.1206 | 0.5900                |                          |
| 0.2000         | 0.8000| 1.2001 | 0.8400                |                          |
| 0.3000         | 0.7000| 1.2515 | 1.0500                |                          |
| 0.4000         | 0.6000| 1.2888 | 1.0712                |                          |
| 0.4999         | 0.5001| 1.3170 | 1.0039                |                          |
| 0.6000         | 0.4000| 1.3389 | 0.9000                |                          |
| 0.6999         | 0.3001| 1.3567 | 0.7300                |                          |
| 0.8000         | 0.2000| 1.371  | 0.5905                |                          |
| 0.8998         | 0.1002| 1.3835 | 0.3199                |                          |
| 1.0000         | 0.0000| 1.3943 | 0.0000                |                          |

*a Standard uncertainty $u$ are $u(x) = 0.0005$, $u(T) = 0.05$ K, $u(\rho) = 0.001$ g cm$^{-3}$, $u(P) = 0.5$ kPa and combined expanded uncertainties (confidence level, 95%) $U(V^E) = 0.0001$ cm$^3$ mol$^{-1}$. 

**Note:** The table provides experimental densities and excess molar volumes for the mixture of MEA (2) and sulfolane (3) at different temperatures and compositions. The uncertainties and conditions under which these measurements were made are also specified.
### $T = 323.15 \text{ K}$

| $a$ | $b$ | $c$ | $d$ |
|-----|-----|-----|-----|
| 0.5999 | 0.4001 | 1.1273 | 0.1141 |
| 0.6999 | 0.3001 | 1.1005 | 0.0700 |
| 0.8000 | 0.2000 | 1.0709 | 0.0262 |
| 0.8999 | 0.1001 | 1.0381 | -0.0199 |
| 1.0000 | 0.0000 | 1.0040 | 0.0000 |

### $T = 333.15 \text{ K}$

| $a$ | $b$ | $c$ | $d$ |
|-----|-----|-----|-----|
| 0.0000 | 1.0000 | 1.2440 | 0.0000 |
| 0.0999 | 0.9001 | 1.2247 | 0.2029 |
| 0.2001 | 0.7999 | 1.2058 | 0.2683 |
| 0.3001 | 0.6999 | 1.1865 | 0.2550 |
| 0.3999 | 0.6001 | 1.1655 | 0.2450 |
| 0.4999 | 0.5001 | 1.1429 | 0.2173 |
| 0.5999 | 0.4001 | 1.1184 | 0.1753 |
| 0.6999 | 0.3001 | 1.0917 | 0.1201 |
| 0.8000 | 0.2000 | 1.0623 | 0.0597 |
| 0.8999 | 0.1001 | 1.0297 | -0.0015 |
| 1.0000 | 0.0000 | 0.9923 | 0.0000 |

### $T = 343.15 \text{ K}$

| $a$ | $b$ | $c$ | $d$ |
|-----|-----|-----|-----|
| 0.0000 | 1.0000 | 1.2354 | 0.0000 |
| 0.0999 | 0.9001 | 1.2156 | 0.2448 |
| 0.2001 | 0.7999 | 1.1966 | 0.3186 |
| 0.3001 | 0.6999 | 1.1773 | 0.3050 |
| 0.3999 | 0.6001 | 1.1563 | 0.2953 |
| 0.4999 | 0.5001 | 1.1337 | 0.2681 |
| 0.5999 | 0.4001 | 1.1093 | 0.2200 |
| 0.6999 | 0.3001 | 1.0828 | 0.1527 |
| 0.8000 | 0.2000 | 1.0537 | 0.0750 |
| 0.8999 | 0.1001 | 1.0213 | 0.0048 |
| 1.0000 | 0.0000 | 0.9841 | 0.0000 |

$^a$ Standard uncertainty $u$ are $u(x) = 0.0005$, $u(T) = 0.05 \text{ K}$, $u(\rho) = 0.001 \text{ g cm}^{-3}$, $u(\eta) = 5\%$, $u(P) = 0.5 \text{ kPa}$ and combined expanded uncertainties (confidence level, 95%) $U(V_E) = 0.0001 \text{ cm}^3 \text{ mol}^{-1}$. 

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7
Fig. 3: Density of [BMIM][NTf₂] (1) + MEA (2) binary mixtures against concentration at various temperatures; (●) 303.15 K; (○) 313.15 K; (▼) 323.15 K; (▲) 333.15 K; (■) 343.15 K.

Fig. 4: Density of MEA (2) + sulfolane (3) binary mixtures against composition at various temperatures; (●) 303.15 K; (○) 313.15 K; (▼) 323.15 K; (▲) 333.15 K; (■) 343.15 K.

3.2 Excess Molar Volume.

Excess molar volume \(V^E\) were calculated based on experimental density of the mixture, \(\rho\), density of the pure component, \(\rho_i\), the corresponding mole fraction, \(x_i\), and molar masses, \(M_i\), using the following Equation 2 [24]

\[
V^E = x_1M_1\left(\frac{1}{\rho} - \frac{1}{\rho_1}\right) + x_2M_2\left(\frac{1}{\rho} - \frac{1}{\rho_2}\right)
\]

where \(x_1, \rho_1\) and \(M_1\) relate to the first component, whereas \(x_2, \rho_2\) and \(M_2\) relate to the second component of the binary mixtures.
Table 3 and Table 4 summarized excess molar volume values and represented by Fig. 5 and Fig. 6 using a Redlich-Kister Equation 3 [25] where \( Y^E \) represent the excess properties:

\[
Y^E = x_1 x_2 \sum_{i=0}^{n} A_i (2x_1 - 1)^i
\]

where \( A_i \) refers to the adjustable parameter and \( n \) is the number of coefficients in the equation. The adjustable parameters, \( A_i \), are summarized in Table 5 and Table 6, respectively.

Fig. 5 shows that the \( V^E \) values for [BMIM][NTf₂] (1) + MEA (2) binary mixtures are positive over the entire mol fraction range of [BMIM][NTf₂] at various temperatures with the maximum of the asymmetric curve at \( x_1 = 0.4 \) mol [BMIM][NTf₂] for all temperatures range. The positive excess molar volume indicates an expansion in volume of the mixture with possible breakdown of the self-associated molecules. Disruption of the closely associated MEA multimers on addition of [BMIM][NTf₂] and formation of new association between the unlike [BMIM][NTf₂] and MEA molecules. Similarly, Fig. 6 shows positive \( V^E \) values for MEA (2) + sulfolane (3) binary mixtures over the entire mol fraction range of composition at various temperatures with the maximum asymmetric curve at \( x_2 = 0.2 \) MEA for all temperatures range. The positive excess molar volume indicates an expansion in volume of the mixture with possible breakdown of the self-associated molecules. Disruption of the closely associated MEA multimers on addition of sulfolane and formation of new association between the unlike MEA and sulfolane molecules. The excess molar volume data for [BMIM][NTf₂] (1) + MEA (2) and MEA (2) + sulfolane (3) binary mixtures were correlated using a Redlich-Kister equation as represented in Equation 3. The adjustable parameters, \( A_i \), are summarized in Table 5 and Table 6, respectively.

Fig. 5: Excess molar volume of [BMIM][NTf₂] (1) + MEA (2) binary mixtures against temperature as function of [BMIM][NTf₂] mol fraction; (⚫)\( T = 303.15 \) K, (○)\( T = 313.15 \) K, (▼)\( T = 323.15 \) K, (△)\( T = 333.15 \) K, (■)\( T = 343.15 \) K
Fig. 6: Excess molar volume of MEA (2) + sulfolane (3) binary mixtures against temperature as function of sulfolane mol fraction; (●) T = 303.15 K, (○) T = 313.15 K, (▲) T = 323.15 K, (△) T = 333.15 K, (■) T = 343.15 K

Table 5: Redlich-Kister fitting coefficients $A_i$ of the $V^E$ of [BMIM][NTf$_2$] (1) + MEA (2) binary mixtures as a function of various temperatures along with their fitting deviations, $\sigma$

| $T / K$ | $A_0$  | $A_1$  | $A_2$  | $A_3$  | $A_4$  | $R^2$  | $\sigma^2$ |
|---------|--------|--------|--------|--------|--------|--------|------------|
| 303.15  | 2.0569 | -0.7691| -0.0835| 3.1342 | 0.2938 | 0.9995 | 0.0056     |
| 313.15  | 3.2035 | -0.4493| 1.0760 | 6.6596 | 1.4246 | 0.9993 | 0.0113     |
| 323.15  | 2.4946 | -0.5052| 0.0721 | 2.3582 | -1.1761| 0.9975 | 0.0153     |
| 333.15  | 2.6907 | -0.8461| 0.2010 | 2.7630 | -1.6736| 0.9979 | 0.0153     |
| 343.15  | 4.0521 | -1.6991| 0.8954 | 0.1423 | 0.9860 | 0.9974 | 0.0257     |

Table 6: Redlich-Kister fitting coefficients $A_i$ of the $V^E$ of MEA (2) + sulfolane (3) binary mixtures as a function of various temperatures along with their fitting deviations, $\sigma$

| $T / K$ | $A_0$  | $A_1$  | $A_2$  | $A_3$  | $A_4$  | $R^2$  | $\sigma^2$ |
|---------|--------|--------|--------|--------|--------|--------|------------|
| 303.15  | 0.2244 | -0.3000| 0.1413 | -0.1204| -1.224 | 0.9938 | 0.0054     |
| 313.15  | 0.5480 | -0.4700| 0.3303 | -0.6856| -0.6250| 0.9986 | 0.0050     |
| 323.15  | 0.8602 | -0.6311| 0.3123 | -1.2358| 0.1936 | 0.9990 | 0.0044     |
| 333.15  | 1.0628 | -0.6893| 0.2124 | -1.5481| 0.5051 | 0.9994 | 0.0043     |
| 343.15  | 0.9669 | -0.5716| 0.2080 | -0.8300| -0.4100| 0.9970 | 0.0077     |

3.3 COSMO-RS modelling

3.3.1 $\sigma$-profile and $\sigma$-potential

For further understanding of the molecular interaction in [BMIM][NTf$_2$] (1) + MEA (2) and MEA (2) + sulfolane (3) binary mixtures, a 3D polarized charged distribution ($\sigma$, sigma) on the molecular surface of the individual components resulted from the quantum chemical calculation were generated using COSMO-RS model. The 3D screening charge distribution on the molecular surface were visualized using a histogram $\sigma$-profile, which used to qualitatively describe the molecule and predict the possible interaction of the components in liquid mixture [26]. The $\sigma$-profile histogram is divided into 3 main regions; hydrogen bond donor region ($\sigma < -0.0082$ e/Å$^2$), hydrogen bond acceptor region ($\sigma > 0.0082$ e/Å$^2$) and non-polar region ($-0.0082 < \sigma < 0.0082$ e/Å$^2$). Fig. 7 shows the $\sigma$-profile and $\sigma$-potential of [BMIM]$^+$ cation, [NTf$_2$]$^-$ anion, MEA and sulfolane molecules.
Fig. 7: \(\sigma\)-profile (a) and \(\sigma\)-potential (b) of [BMIM]\(^+\) cation, [NTf\(_2\)]\(^-\) anion, MEA and sulfolane predicted by COSMO-RS model.

Fig 8 shows \(\sigma\)-profile and \(\sigma\)-potential for [BMIM]\(^+\) cation, [NTf\(_2\)]\(^-\) anion, MEA and sulfolane generated by COSMO-RS model. \(\sigma\)-profile for [BMIM]\(^+\) cation is dominated by a main peak at \(-0.004\) e/Å\(^2\) in the non-polar region of the histogram illustrates the aliphatic alkyl chain and the aromatic head group (green), while \(-0.009\) e/Å\(^2\) peak in the hydrogen bond donor region indicates the acidic hydrogen atom of the aromatic ring (blue). Prominent peak at \(+0.003\) e/Å\(^2\) in the [NTf\(_2\)]\(^-\) anion \(\sigma\)-profile illustrates the the non-polar fluorinated alkyl group (green), while the \(+0.011\) e/Å\(^2\) peak in the hydrogen bond acceptor region indicates the polar sulfonyl group (red). \(\sigma\)-potential shows a negative value \(\sigma > 0.0082\) e/Å\(^2\) for [BMIM]\(^+\) cation which indicates an affinity to a hydrogen bond acceptor while a negative value at \(\sigma < -0.0082\) e/Å\(^2\) for [NTf\(_2\)]\(^-\) anion exhibits an affinity toward hydrogen bond donor.
The σ-profile of MEA illustrates peaks in both H-bond donor groups and hydrogen bond acceptor region which illustrates amphoteric behavior, highlighting their ability to act as H-bond acceptors and donor. A peak at -0.009 e/Å² is attributed to the polar hydrogen of the hydroxyl and an amine group (blue). MEA molecule displays multiple peaks in the hydrogen bond acceptor region arising from the lone pair of the oxygen atom of the hydroxyl group as well as the lone pair of the nitrogen atom of the amine group (red). Non-polar peak at -0.005 e/Å² indicates the C-C backbone of the ethanolamine molecule.

MEA displays a negative at both σ < -0.0082 e/Å² and σ > 0.0082 e/Å² which indicates affinity to both hydrogen bond donor and hydrogen bond acceptor. Hence, self-association might be favorable interactions between the MEA molecules.

In Fig. 8, σ-profile for sulfolane presents a peak at +0.012 e/Å² which is assigned to the sulfonyl group (red) identified as hydrogen bond acceptor. Peak at -0.006 e/Å² within the non-polar region is identified as four-carbon ring bonded to the sulfur atom (green). σ-potential for sulfolane presents a negative value at σ < -0.0082 e/Å² which indicates an affinity to a hydrogen bond donor and a positive value at σ > 0.0082 e/Å² corresponds with no affinity to hydrogen bond acceptor. From the overall analysis of the σ-profile of sulfolane, a distribution charge on the σ polarity scale around hydrogen bond acceptor region indicates the ability of sulfolane to act as a base. Hence it is possible to forecast that component with hydrogen bond donor groups (acidic character) able to develop a favorable intermolecular interaction with sulfolane. Furthermore, sulfolane is shown to possess high dipole moment due to presence of only H-bond acceptor region in the molecule.

σ-profile and σ-potential for [BMIM]^+ and [NTf₂]⁻ show an H-bond donor and H-bond acceptor, respectively the complement each of the ion pairs. Both [BMIM]^+ cation and [NTf₂]⁻ anion show a peak in the non-polar region. On the other hand, σ-profile and σ-potential for sulfolane shows an H-bond acceptor characteristic. While, σ-profile and σ-potential show MEA has an amphoteric characteristic with both H-bond donor and H-bond acceptor present in the molecule suggesting intramolecular H-bonding with each MEA molecule. Introduction of [BMIM][NTf₂] or sulfolane into the MEA matrix would cause disruption to the intramolecular H-bond the leads to expansion of volume. MEA has an amphoteric characteristic with both H-bond donor and H-bond acceptor present in the molecule. This suggests a strong intramolecular H-bonding with each MEA molecule. On the other hand, sulfolane present with an H-bond acceptor which may break the existing MEA intramolecular H-bonding which lead to expansion of mixture volume. Similarly, presence of peak in the non-polar region in both molecules with sulfolane exhibit a prominent peak in non-polar region at -0.006 e/Å² with higher intensity than MEA non-polar peak. This indicates the possibility of weak van der Waal’s interaction predominates in these binary mixtures.

**Conclusion**

In this research, we conduct a density measurement for binary mixtures of [BMIM][NTf₂] (1) + MEA (2) and MEA (2) + sulfolane (3) at whole range of composition and temperature ranging from 303.15 to 343.15 K. Based on the experimental data, excess molar volume was calculated. Both binary mixtures of [BMIM][NTf₂] (1) + MEA (2) and MEA (2) + sulfolane (3) exhibit a positive value in excess molar volume due to expansion of volume and negative viscosity deviation values indicating for a weak interaction between MEA and [BMIM][NTf₂] or sulfolane components. This observation is primarily due to the breakage of the intramolecular hydrogen bond between MEA molecules via the introduction of [BMIM][NTf₂] or sulfolane components. This behavior of the binary solutions is justified using COSMO-RS based on the σ-profile and σ-potential of each of the component.

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Acknowledgments
The author would like to express acknowledgment to Universiti Malaya for granting this project under Universiti Malaya Research Grant UMRG (RP006F-13SUS) and Postgraduate Research Fund (PG102-2013A). Our sincere appreciations are also extended to University of Malaya Centre of Ionic Liquids (UMCiL).